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HAEGGSTRÖM, Jesper, Z. [/]; (). NORDLUND, Pär [/]; (). THUNISSEN, Marjolein [/]; (). HAEGGSTRÖM, Jesper, Z. [/]; (). NORDLUND, Pär [/]; (). THUNISSEN, Marjolein [/]; (). BERG, S., A.; ().

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(54) Title: DRUG DESIGN BASED ON THE STRUCTURE OF LTA; 4 HYDROLASE

(54) Titre: CONCEPTION DE MEDICAMENTS BASES SUR LA STRUCTURE DE LA LTA¿4-HYDROLASE

(57) Abstract

The present invention relates to an isolated leukotriene A¿4 (LTA¿4) hydrolase, which LTA¿4 hydrolase is present in its naturally ocurring three dimensional form. It is the first three-dimensional structure of any protein component of the leukotriene cascade and enables a description of the structural basis and molecular mechanisms for the two catalytic activities of LTA¿4 hydrolase. Further, the invention also relates to LTA¿4 hydrolase complexed with an inhibitor. The structural information provided by the present invention will make possible rational design of enzyme inhibitors, which may be developed into clinically useful anti-inflammatory drugs.

(57) Abrégé

Cette invention se rapporte à une leucotriène A¿4 (LTA¿4)-hydrolase isolée, qui est présente sous sa forme tridimensionnelle existant à l'état naturel. C'est la première structure tridimensionnelle d'un composant protéinique de la cascade de leucotriène et elle permet une description de la base structurelle et des mécanismes moléculaires pour les deux activités catalytiques de la LTA¿4-hydrolase. Cette invention se rapporte en outre à une LTA¿4-hydrolase formant complexe avec un inhibiteur. Les informations structurelles fournies par cette invention vont permettre une conception rationnelle d'inhibiteurs enzymatiques, qui peuvent être mis au point sous la forme de médicaments anti-inflammatoires utiles sur le plan clinique.

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DRUG DESIGN BASED ON THE STRUCTURE OF LTA₄ HYDROLASE 1. BACKGROUND

1.1 Technical field

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The present invention relates to methods of design or identification of biologically active compounds, which methods are based on the first definition ever of a three-dimensional structure of a protein involved in the leukotriene cascade. Further, the invention relates to novel compounds obtained by said methods, to advantageous uses of such compounds as well as to processes for the preparation thereof.

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10 <u>1.2 Prior art</u>

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Leukotriene A4 (LTA4) hydrolase is a pivotal enzyme in the biosynthesis of leukotrienes, a family of paracrine hormones implicated in the pathophysiology of inflammatory and allergic disorders, in particular bronchial asthma (Samuelsson, B. Science 220, 568-75 (1983); and Lewis, R.A., Austen, K.F. & Soberman, R.J. N Engl J Med 323, 645-55 (1990)). Leukotrienes are formed by immunocompetent cells including neutrophils, eosinophils, basophils, mast cells, and macrophages, in response to a variety of immunological as well as non-immunological stimuli. These lipid mediators are divided into two major classes exemplified by the chemotaxin LTB4, and the spasmogenic cysteinyl-leukotrienes (LTC4, LTD4, and LTE4). Leukotriene biosynthesis is initiated by the enzyme 5-lipoxygenase which converts arachidonic acid into the unstable epoxide LTA4, a central intermediate in the leukotriene cascade. LTA4 may in turn be hydrolyzed into LTB4 by the enzyme LTA4 hydrolase, or conjugated with GSH to form LTC4, a reaction catalyzed by a specific LTC4 synthase. During cellular activation, all key enzymes in leukotriene biosynthesis, except LTA4 hydrolase, form a biosynthetic complex assembled at the nuclear membrane, suggesting that leukotrienes may have unknown intranuclear functions related to gene regulation or cell growth (Serhan, C.N., Haeggstrom, J.Z. & Leslie, C.C. Faseb J 10, 1147-58 (1996)).

Leukotriene B4, the natural product of LTA4 hydrolase, is one of the most powerful chemotactic agents known to date and triggers leukocyte adherence and ag-

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M.V., Shipley, M.E. & Smith, M.J.H. Nature 286, 264-265 (1980)). Hence, this molecule is regarded as a key mediator of inflammation, and has been implicated in a number of diseases, including arthritis, psoriasis, inflammatory bowel disease (IBD), and chronic obstructive pulmonary disease (COPD). Furthermore, the role of LTB4 in inflammation has been well corroborated by the anti-inflammatory properties of LTA4 hydrolase inhibitors, particularly in combination with a cyclooxygenase inhibitor, and specific LTB4 receptor antagonists, as well as the reduced inflammatory reactions observed in several animal models of leukotriene deficiency (Tsuji, F., Miyake, Y., Enomoto, H., Horiuchi, M., Mita, S. Eur. J. Pharmacol. 346, 81-85, (1998); Chen, X.S., Sheller, J.R., Johnson, E.N. & Funk, C.D. Nature 372, 179-182 (1994); Griffiths, R.J., et al. Proc Natl Acad Sci USA 92, 517-21 (1995); and Griffiths, R.J., et al. J Exp Med 185, 1123-9 (1997)). In addition, LTB4 modulates the immune response, e.g., by interference with specific subsets of lymphocytes, production of cytokines, as well as liberation of immunoglobulins from B-lymphocytes (Payan, D.G., Missirian-Bastian, A. & Goetzl, E.J. Proc Natl Acad Sci USA 81, 3501-5 (1984); Rola-Pleszczynski, M. & Lemaire, I. J. Immunol 135, 3958-61 (1985); and Yamaoka, K.A., Claesson, H.E. & Rosen, A. J Immunol 143, 1996-2000 (1989)). Recent data also indicate that LTB4 stimulates, and thus has a crucial role in the regulation of, cell proliferation and cell survival in HL-60 cells, suggesting that LTA4 hydrolase inhibitors may have an anti-proliferative effect. (Dittman, K.H., Mayer, C., Rodemann, H.P., Petrides, P.E., and Denzlinger, C. Leuk. Res. 22, 49-53 (1998)). The cell surface receptor for LTB4 (BLTR) was recently cloned and found to be abundantly expressed in the immune system, including lymphocytes, spleen and thymus (Yokomizo, T., Izumi, T., Chang, K., Takuwa, Y. & Shimuzu, T. Nature 387, 620-624 (1997)). BLTR belongs to a family of chemokine receptors and, interestingly, together with CD4 it was found to be an efficient coreceptor for HIV-1 infection (Owman, C., et al. Proc Natl Acad Sci USA 95, 9530-4 (1998)). Moreover, LTB4 is also a natural ligand to the nuclear orphan receptor PPARa.

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gregation at only nM concentrations (Ford-Hutchinson, A.W., Bray, M.A., Doig,

suggesting that LTB4 may have intranuclear functions possibly related to lipid homeostasis (Devchand, P.R., et al. Nature 384, 39-43 (1996)).

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LTA4 hydrolase is a cytosolic 69 kDa enzyme without any similarity to other soluble or membrane bound xenobiotic epoxide hydrolases (Funk, C.D., et al. Proc Natl Acad Sci U S A 84, 6677-81 (1987)). The enzyme's epoxide hydrolase activity, which generates LTB4, is highly substrate selective accepting only LTA4 and to a small extent the double bond isomers LTA3 and LTA5. Typically, LTA4 hydrolase undergoes suicide inactivation and covalent modification when exposed to LTA4 (Evans, J.F., Nathaniel, D.J., Zamboni, R.J. & Ford-Hutchinson, A.W. J. Biol. Chem. 260, 10966-10970 (1985)). During this process, LTA4 apparently binds to Tyr-378, a residue which also seems to play a role for the formation of the critical cis-trans-trans geometry in the conjugated triene structure of LTB4 (Mueller, M.J., et al. Proc Natl Acad Sci U S A 93, 5931-5935 (1996); and Mueller, M., Andberg, M., Samuelsson, B. & Haeggstrom, J. Z. J. Biol. Chem. 271, 24345-24348 (1996)).

From sequence comparisons with certain metalloproteases and aminopeptidases, a zinc binding motif (HEXXH-X18-E) was unexpectedly found in LTA4 hydrolase (Vallee, B.L. & Auld, D.S. Proc. Natl. Acad. Sci. USA 87, 220-224 (1990)). Further studies demonstrated that the enzyme indeed contains one catalytic zinc atom complexed to His295, His299, and Glu318 (Medina, J.F., et al. Proc. Natl. Acad. Sci. USA 88, 7620-7624 (1991)). In addition, a previously unknown peptide cleaving activity was discovered which requires the presence of anions, particularly chloride (Haeggström, J.Z., Wetterholm, A., Medina, J.F. & Samuelsson, B. J Lipid Mediator 6, 1-13 (1993)). Although the endogenous physiological peptidase substrate(s) has not yet been identified, LTA4 hydrolase cleaves certain arginyl di- and tripeptides with very high efficiency (Örning, L., Gierse, J.K. & Fitzpatrick, F.A. J. Biol. Chem. 269, 11269-11273 (1994)). Hence, LTA4 hydrolase can be described as a bifunctional zinc metalloenzyme with the unique ability to accept both lipid and peptide substrates. Using site-directed mutagenesis, Glu296 and Tyr383 were found to be critical for the peptidase reaction, presumably as a general base and proton donor, respectively (Blomster, M., Wetterholm, A., Mueller, M.J. & Haeggström,

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J.Z. Eur. J. Biochem. 231, 528-534 (1995); and Wetterholm, A., et al. Proc Natl Acad Sci U SA 89, 9141-9145 (1992)). Since the enzyme's ability to convert LTA4 into LTB4 was not affected by the mutations, the two enzyme activities of LTA4 hydrolase are exerted via non-identical but overlapping active sites. Notably, unlike other enzymes in the leukotriene cascade, LTA4 hydrolase is ubiquitous in mammalian cells and tissues suggesting that it may have other functions presumably related to its peptide cleaving activity.

As a consequence of the identification of LTA₄ hydrolase as a zinc metalloenzyme with a peptidase activity, it was observed that LTA₄ hydrolase is inhibited by bestatin, a general aminopeptidase inhibitor, and captopril, an inhibitor of angiotensin converting enzyme (Örning, L., et al. J. Biol. Chem. 266, 16507-16511 (1991)).

Tsuge et al., (J. Mol. Biol. 238,854-856 (1994)), have described the crystallization of LTA₄ hydrolase. However, despite the well recognized need thereof, the three-dimensional structure of LTA₄ hydrolase has not yet been disclosed. More specifically, the problems that need to be overcome in order to provide such a determination may in brief be explained as follows. There are two major difficulties in obtaining a three-dimensional structure of a protein molecule. The first one is to grow crystals of good quality that are reproducible and diffract to atomic resolution (beyond 2.5Å). This means a thorough and cumbersome investigation of parameters that influence the crystal growth such as pH, temperature, nature of buffers, nature of precipitant, just to mention a few. The addition of ligands such as substrate analogues or inhibitors or the addition of other molecules can be important for obtaining good crystals. There is only little understanding of the physical background of the crystallisation process which means that the search for suitable crystallisation conditions for a certain protein is unique, requires creativity and intuition, and is governed by trial and error procedures. The purity of the protein is also a crucial parameter in the crystallisation and a suitable degree of purity can be hard, or even imposible, to achieve. The second major difficulty is associated with overcoming the phase-problem which is inherent to X-ray diffraction methods. To be able to overcome this problem it is necessary to substitute the protein with suitable heavy

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atom substance such as e.g. mercury, gold or platinum compounds. Crystals often cannot withstand the treatment with these compounds and the search for suitable substitutions is not straight forward and may become very exhaustive. Another option is to substitute all methionines by seleno-methionine (Se-Met) residues. This method requires production of recombinant protein in special strains of E. coli under non-standard conditions, followed by a new purification and recrystallisation of the Se-Met containing protein. Although Tsuge et al reported the crystallisation of LTA4 hydrolase, their crystals only diffracted to medium resolution and the phaseproblem was not solved. Thus, as a reliable definition of the three-dimensional structure of LTA₄ hydrolase would enable e.g. a display in visual form on a computer screen of the shape of the molecule, then, could the above mentioned problems be solved, a whole range of possibilities would be opened, such as rational structure-based drug design, e.g. in combination with combinatorial chemistry, aimed at production of novel medicaments useful in disorders associated with the leukotriene cascade, as well as protein-engineering to create novel variants of the enzyme with altered, but yet useful, catalytic properties.

As LTA4 hydrolase is a recognized important drug target, some inhibitors thereof have been synthesized (Wetterholm, A., et al. J Pharmacol Exp Ther 275, 31-7 (1995); and Yuan, W., Wong, C., Haeggstrom, J. Z., Wetterholm, A. & Samuelsson, B. J. Am. Chem. Soc., 114, 6552-6553 (1992)). Interestingly, certain inhibitors of LTA4 hydrolase were reported to act also as LTB4 receptor antagonists (Labaudinière R, Hilboll G, Leon-Lomeli A, Terlain B, Cavy F, Parnham M, Kuhl P, and Dereu N. J. Med. Chem. 35, 3170-3179 (1992)). Due to the absence of any available information regarding the three-dimensional structure of LTA4 hydrolase, as discussed above, none of the previously described inhibitors have been designed based on the exact structure thereof. Accordingly, there is a need within this field of determining the three-dimensional structure of LTA4 hydrolase in order to design more potent and selective inhibitors of LTA4 hydrolase as well as modified structures exhibiting even more advantageous pharmaceutical properties.

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5 2. THE PRESENT INVENTION As the following chapter includes a substantial amount of text, it has herein been divided into separate sections, each one of which disclose separate aspects of the present invention. 10 5 **Index Chapter 2** 2.1 Summary of the invention 15 2.2 Brief description of the drawings 2.3 Definitions 10 2.4 Detailed description of the invention 20 2.4.1 LTA₄ hydrolase, subsequences and analogues thereof 2.4.2 Compounds complementary to LTA₄ hydrolase 2.4.3 A complex of LTA₄ hydrolase and acomplementary compound 25 2.4.4 Advantageous uses of LTA₄ hydrolase, complementery compounds and 15 complexes thereof 2.4.5 Screening for LTA₄ hydrolase analogues 2.4.5 (a) Method 30 2.4.5 (b) Analogues obtainable by the present screening method 2.4.5 (c) Mutated forms of LTA₄ hydrolase obtainable by the present screening 20 method 35 2.4.5 (d) Nucleic acids encoding the novel compounds 2.4.6 (a) Production and purification of genetically modified forms of LTA₄ hydrolase 40 2.4.6 (b) Purified LTA₄ hydrolase 25 2.4.7 Identification of LTA₄ hydrolase binding compounds 2.4.7 (a) Method 45 2.4.7 (b) Identified binding compounds 2.4.8 Protein engineering 2.4.8 (a) Method 50 30 2.4.8. (b) Novel specifically designed proteins 2.4.8. (c) Use of genetically modified LTA₄ hydrolase

5		2.4.9 Pharmaceutical applications of the present invention
		2.4.9 (a) First medical indication
		2.4.9 (b) Second medical indication and pharmaceutical methods
10		2.4.9.(c) Methods of treatment
	5	2.5 Production of the novel molecules
		2.6 Detailed description of the drawings
15		2.1 Summary of the invention
		The object of the present invention is to fulfill the above defined need. This has
		been achieved by the crystallization and determination of the three-dimensional
20	10	structure of LTA4 hydrolase complexed with the competitive inhibitor bestatin and
20		subsequent structure determination of complexes between LTA ₄ hydrolase and two
		specific inhibitors. It is the first three-dimensional structure of any protein compo-
		nent of the leukotriene cascade and enables a description of the structural basis and
25		molecular mechanisms of various enzyme functions, such as the two catalytic acti-
	15	vities of LTA4 hydrolase. In addition, the structural information will now make pos-
		sible rational design of enzyme inhibitors, which may be developed into clinically
30		useful anti-inflammatory drugs.
		2.2 Brief description of the drawings
		Figure 1 shows the key enzymes and intermediates in leukotriene biosynthesis.
35	20	Figure 2 shows 2Fo-Fc density contoured at 1.1 s. Part of the active site in the
		neighborhood of the bestatin molecules is shown.
		Figure 3 is a ribbon diagram of the tertiary structure of leukotriene A4 hydrolase.
40		Figure 4 shows ribbon diagrams of the N-terminal domains of . LTA ₄ hydrolase.
		Figure 5 shows ribbon diagrams of the catalytic domain of LTA ₄ hydrolase and the-
	25	rolysin.
45		Figure 6 shows the structure of the C-terminal domain.
		Figure 7 illustrates zinc binding ligands in LTA4 hydrolase.
		Figure 8 (a) is a Ball-and-Stick presentation of the binding of bestatin in LTA4 hyd-
50		rolase, while Figure 8 (b) is a schematic overview of bestatin binding in LTA4 hyd-
50	30	rolase.

5 Figure 9 (a) is a wire representation of the central cavity found in LTA4 hydrolase (shown as $C\alpha$ -trace). Figure 9 (b) is a schematic presentation for the proposed binding of LTA4 into the 10 cavity. Figure 10 is a schematic representation for the proposed reaction mechanism of the 5 epoxide hydrolase. 2.3 Definitions 15 In the present context, the term "the three-dimensional form adopted thereof in nature" is to be understood as the conformational structure, defined by the parameters x, y and z in a conventional coordinate system, that a naturally occurring mole-10 20

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The specific conditions during which the herein presented data were collected are detailed in the section "Experimental".

cule adapt under conditions where it is capable of exerting its biological activities.

The term "isolated" and variations thereof when used in connection with a molecule, such as protein, a polypeptide or a nucleic acid, means that said molecule is isolated from other substances, such as other proteins, DNA etc normally accompanying it in its natural environment.

The term "leukotriene A₄ (LTA₄) hydrolase" as used herein is to be understood to include any mammalian or other LTA₄ hydrolase which comprises the same backbone as the human form specifically disclosed in the present application, irrespective of source. The amino acid sequences of mammalian LTA₄ hydrolase have been shown to be identical to about 90%. Thus, the three-dimensional structures thereof may be suspected to be identical to approximately the same extent.

"Thiolamine" and "hydroxamic acid" are used herein to denote the compounds examplified in the Experimental section of the present specification.

A "complementary compound" means any compound, the structure of which enables a binding thereof to a specified protein, i.e a compound having a conformation or structure enabling such a suitable fit as to provide an energetically favorable interaction between protein-complementary compound.

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"Analogue" means, as used herein, a chemically altered molecule which shares the backbone with, or at least structurally resembles, a "parent molecule". In the present specification, such a "parent molecule" may be LTA₄ hydrolase or an inhibitor thereof.

In the present application, the term "active site" is to be understood to include any region capable of binding a substrate and converting it into product.

The term "nucleic acid" refers to a deoxyribonucleotide or ribonucleotide polymer in either single- or double-stranded form, and unless otherwise limited, encompasses known analogs of nucleotides, that can function in a similar manner as naturally occurring nucleotides.

The phrase "hybridising specifically to" refers to the binding, duplexing, or hybridising of a molecule only to a particular nucleotide sequence under stringent conditions when that sequence is present in a complex mixture (e.g., total cellular) of DNA or RNA. The term "stringent conditions" refers to conditions under which a probe will hybridise to its target subsequence, but to no other sequences. Stringent conditions are sequence-dependent and will be different in different circumstances. Longer sequences hybridise specifically at higher temperatures. Generally, stringent conditions are selected to be about 5°C lower than the thermal melting point Tm for the specific sequence at a defined ionic strength and pH. The Tm is the temperature (under defined ionic strength, pH, and nucleic acid concentration) at which 50% of the probes complementary to the target sequence hybridise to the target sequence at equilibrium. (As the target sequences are generally present in excess, at Tm, 50% of the probes are occupies at equilibrium). Typically, stringent conditions will be those in which the salt concentration is less than about 1.0 M Na ion, typically about 0.01 to 1.0 M Na ion concentration (or other salts) at pH 7.0 to 8.3 and the temperature is at least about 30°C for short probes (e.g., 10 to 50 nucleotides) and at least about 60°C for long probes (e.g., greater than 50 nucleotides). Stringent conditions may also be achieved with the addition of destabilizing agents such as formamide.

"Essentially pure" means herein a purity of at least about 80%, especially at least about 90% and preferably at least about 95%, such as 98-99%. The purity of

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LTA₄ hydrolase, an analogue or inhibitor thereof is according to the present invention preferably determined by general biochemical and biophysical methods well-known to the skilled in this field. For proteins, SDS polyacrylamide gel electrophoresis (SDS-PAGE) with Coomassie and silver staining or amino acid sequence analysis can be used, whereas high-pressure liquid chromatography (HPLC), gas chromatography coupled to mass spectrometry (GC-MS), and nuclear magnetic resonance spectroscopy (NMR) are suitable methods for small organic molecules (peptides, lipids, or carbohydrates, or combinations of these classes of substances).

2.4 Detailed description of the invention

2.4.1 LTA₄ hydrolase, subsequences and analogues thereof

In a first aspect, the present invention relates to an isolated protein comprising at least a subsequence of the amino acid sequence of leukotriene A₄ (LTA₄) hydrolase, which subsequence has the corresponding three-dimensional form adopted thereof in nature. The protein according to invention as discussed below and elsewhere in this application is also understood to encompass any other functionally equivalent part, derivative or conformational analogue thereof. More specifically, the invention relates to the above disclosed protein which comprises a subsequence of the amino acid sequence of leukotriene A₄ (LTA₄) hydrolase, which is able to participate in, and influence, e.g. by providing enzymatic activity, the leukotriene cascade. Most preferably, the protein according to the invention is capable of controling said cascade by exerting an enzymatic activity and thus regulate the production of leukotriene B₄ (LTB₄). In a particular embodiment, the protein is comprised of essentially all of the amino acid sequence of leukotriene A₄ (LTA₄) hydrolase as disclosed in SEQ ID NO 1, or a functionally equivalent part, derivative or conformational analogue thereof.

Thus, the present invention relates to an isolated LTA₄ hydrolase in its naturally occurring three-dimensional form. More specifically, the present application provides a listing illustrating, for the first time, the coordinates defining human LTA₄ hydrolase complexed to an inhibitor thereof. Thus, the coordinates defining the conformation of LTA₄ hydrolase have been determined by the present inventors as com-

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plexed with bestatin, thiolamine and hydroxamic acid, respectively. Bestatin is a universal inhibitor of amino peptidase activity (see e.g. Mathé, G. Biochem. Pharmacol. 45, 49-54 (1991)), while the last mentioned two are specific inhibitors of LTA4 hydrolase. Based on these different activities, said inhibitors may be used as models in the design of novel molecules having desired properties. Methods for such design will be discussed in further detail below as a further advantageous aspect of the invention. For reasons of conveniance for the reader of the present specification, the data collection comprising the novel coordinates according to the invention is included in the present description as a separate section denoted "X-ray data", as Table 9, immediately preceding the claims. In said table, atom no 1 to atom no 4876 define the LTA4 hydrolase part of the complex. (protein part), atom no 4877 refers to Zn, atom nos. 4878-4880 refer to Yb, atom nos. 4881-4885 refer to imidazole, atom nos. 4886-4889 refer to acetate, atom nos 4890-4908 refer to thiolamine while atom nos. 4909-5160 refer to water. Thus, the intervening atoms relate to the metals that bind in LTA4 hydrolase, i.e. the active site Zn atom and the Yb atoms that were crucial for the present structure determination. The conditions prevailing at the determination thereof will be described in detail in the Experimental section below. As the skilled in this field realises, such coordinates usually exhibit a certain degree of variation, due to e.g. thermal motion and slight differences in crystal packing. Thus, any references herein to Table 9 in connection with the proteins and other molecules are merely intended to illustrate an average value for each of the coordinates defining the conformation of the molecules under identical conditions, as determined by use of the same apparatus and method. Accordingly, this embodiment of the invention is not limited to a molecule having exactly the specified coordinates, but rather to molecules capable of adopting such a structure. For example, a human LTA4 hydrolase according to the invention will exhibit a strong bit a conformational similarity with the coordinates presented by atom nos 1 -4876 of Table 9, wherein a variation of about 1%, or 0.5 Å, may be expected. Accordingly, any such variants are within the scope of the present invention.

As regards amino acid sequence, in a specific embodiment, the protein according to the invention is identical, by direct sequence comparison, to at least about

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50%, more specifically, at least about 70%, such as at least about 90%, to the LTA4 10 5

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hydrolase as defined by SEQ ID NO. 1 while in the three-dimensional form adopted thereof in nature. In this context, it is noted that the amino acid sequence of LTA4 hydrolase also appears from the data of Table 9, but is also included as a separate sequence listing for reasons of clarity. The protein of this embodiment of the invention are e.g. variants originating from any species, preferably mammals, such as humans, mice or other rodents, etc. Alternatively, the variants including subsequences of the human sequence are mutated forms, resulting from either spontaneous mutations or deliberately produced mutations, as discussed in more detail below.

One preferred embodiment of the present invention is a protein which comprises at least one of the regions defined below in Tables 1-3 below as active sites.

Table 1: Residues lining the big cavity from outsite to insite

	Left wall	Right wall
1		Lys608, Asp606, Lys605, Lys354, Thr355
2	Phe356, Phe362	Gln544, Asp573, Lys572, Arg568
3	Val376	Lys565, Arg540, Leu507
4	Ser380, Ser352, Glu348	Pro569
5	Тут378, Glu348	Arg563, Glu533, Phe536, Arg537, Tyr267
6	Тут383, Phe314, Glu318, Glu384, Arg326	
7	Gly268, Gly269, Met270	His295, Asn341, Phe340
8	Ser288, His497	Glu325, Asn291

In Table 1, Lys565, Ser380, Pro569, Glu533, Tyr383, Phe314, Glu318, Glu384, Arg326, Gly268, Gly269, Met270, His295, Phe340, Ser288, and Glu325 are strictly conserved amino acids, while Lys608, Phe356, Phe362, Lys572, Arg568, Tyr378,

Phe536, Tyr 267, and Asn291 are conserved in nature.

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5 Table 2: Amino-acids in the bestatin binding site ("basic" amino-peptidase site) The binding of bestatin to LTA4 hydrolase may also be described by way of coordinates. Below follows the specific amino acids involved in the binding of bestatin and similar structures, as defined according to the invention. 10 5 Gln136; Ala137; Tyr267; Gly268; Gly269; Met270; Glu271; Val292; His295; Glu296; His299; Glu318; Tyr378; Tyr383; Arg563; Lys565. 15 Table 3: Amino acids in the leukotriene binding site The present amino acids define the site binding leukotriene-based inhibitors, such as 10 20 thiolamine and hydroxamic acid, as shown in Table 9 for thiolamine. Gln136; Ala137; Tyr267; Gly268; Gly269; Met270; Glu271; Val292; His295; 25 Glu296; His299; Trp315; Glu318; Val322; Phe362; Val367; Leu369; Pro374; 15 Asp375; Ile372; Ala377; Pro382; Tyr378; Tyr383; Arg563; Lys565. 30 In Tables 1-3 above, the enumeration of the amino acid sequence of LTA₄ hydrolase begin without the initial Met. Thus, compared to SEQ ID NO 1, which includes the initial Met, the amino acid enumeration above is lowered by one. Accordingly, 20 Gln136 above corresponds to Gln 137 of SED ID NO 1, Ala137 above corresponds 35 to Ala 138 of SEQ ID NO 1, etc. Table 4: General catalytic domain for the M1 class of enzymes 40 Amino acids no. 210-450. 25 The present region will provide a basis for the development of enzyme inhibitors 45 useful in the control other biological pathways than the leukotriene cascade. Thus, as regards the above defined region of aminopeptidase activity of LTA4 hy-50 30 drolase, the present inventors have surprisingly observed, that said region is in fact universal for all enzymes belonging to the metallohydrolase family denoted M1.

Thus, this specific subsequence of LTA₄ hydrolase is encompassed by the present invention as a novel protein *per se*. In addition to the various advantageous uses of subsequences of LTA₄ hydrolase described herein in connection with the leukotriene cascade, this region, which is shared between all M1 enzymes, will find several further applications in connection with other enzymatic pathways. For example, the present region, herein denoted the "M1 region" in order to clarify that it is shared between the M1 enzymes, may advantageously be used to produce synthetic inhibitors, or identify natural inhibitors, of any one of the other M1 enzymes. Such M1 inhibitors will be discussed below when compounds complementary to LTA₄ hydrolase are disclosed.

The above disclosed proteins and peptides comprising subunits of LTA₄ hydrolase are advantageously used e.g. as enzymes or more preferably in methods wherein novel inhibitors of enzymatic activities are identified and/or designed.

2.4.2 Compounds complementary to LTA₄ hydrolase

In a second aspect, the present invention relates to a novel compound defined by a structure substantially complementary to the above described protein, preferably identified by use of the novel LTA₄ hydrolase conformation according to the present invention. The complementary compound is a naturally occurring or synthetic protein, peptide, lipid, carbohydrate or any other organic or inorganic compound. In relation to naturally occurring compounds, it is to be understood that the present invention relates to such compounds as isolated from their natural environment, preferably identifiable by aid of the novel coordinates defining structures according to the invention, as examplified by the complementary compounds used in the complexes shown in Table 9.

In a first embodiment, the present complementary compound is substantially complementary to an enzymatically active site of the protein and is advantageously capable of specifically inhibiting an enzymatic activity of said protein. Thus, in one embodiment, the present compound is substantially complementary to parts, or all, of the "basic" aminopeptidase binding site defined in Table 2 above. Thus, the pres-

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ent compound is an inhibitor capable of specifically inhibiting an aminopeptidase

activity of an enzyme, preferably of LTA₄ hydrolase. In an alternative embodiment, the present compound is substantially complementary to parts, or all, of the leukotriene binding site as defined in Table 3 above. Thus, the present compound is an inhibitor capable of specifically inhibiting an epoxide hydrolase activity of an enzyme, preferably of LTA₄ hydrolase. (The inhibition of both aminopeptidase and epoxidase hydrolase is discussed in detail below in the experimental section.) As the present two binding sites of LTA₄ hydrolase overlap in part, a further embodiment is a compound which is complementary to essential parts of both of the above discussed two binding sites, in part or partially, which thus preferably is an inhibitor of both the discussed activities.

As already mentioned above, one compound which is complementary to an enzymatically active site of LTA₄ hydrolase is a compound complementary to the M1 region thereof and thus capable of partial or total inhibition of the enzymatic activity of LTA₄ hydrolase or any other metallohydrolase belonging to the M1 family. In the present application, such inhibitors will be denoted M1 inhibitors.

As the skilled in this field will realise, the present inhibitors disclosed above need not be compound that inhibit a biological activity completely, but may be capable of exerting a partially inhibiting activity, i.e, lowering the enzymatic activity.

In another embodiment, the present complementary compound is a compound which is also capable of binding to the receptor for the product of an LTA₄ hydrolase, i.e. an LTB₄ receptor, e.g. on a cell, such as a polymorphonuclear leukocyte. Thus, such a compound may be useful as an LTB₄ antagonist whereby the biological effect of LTA₄ hydrolase activity may be regulated. Accordingly, any such LTB₄ antagonist designed and/or identified using the coordinates of LTA₄ hydrolase as presented herein are also encompassed by the present invention.

In another embodiment, the present complementary compound is a compound which, apart from being capable of binding to an active site of LTA4 hydrolase, is also capable of binding to an active site of LTC4 synthase which binds the same substrate as LTA4 hydrolase, i.e. LTA4, and turns it over into LTC4 (cf. Fig 1) and

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is thus expected to share important structural features with the active site of LTA4 hydrolase. Such a compound may be useful as an inhibitor of LTC4 biosynthesis, whereby the production thereof may be regulated. Accordingly, any such LTC4 synthase inhibitor, designed and/or identified using the coordinates of LTA4 hydrolase, are also encompassed by the present invention.

The specific properties and advantageous uses of the present compounds as well as the design and production of novel LTA₄ hydrolase inhibitors will be described in further detail below in relation to the various methods.

2.4.3 A complex of LTA₄ hydrolase and a complementary compound

In a third aspect, the present invention relates to an isolated complex comprised of a protein as described above and a compound complementary to said protein. Said complementary compound may thus be an inhibitor of one or more of the protein's enzymatic activities, such as an aminopeptidase and/or epoxide hydrolase activity, such as bestatin, hydroxamic acid or thiolamine, or leukotriene B4 or any analogue thereof, or LTC₄ or any analogue thereof. Examples of complementary compounds are bestatin, thiolamine or hydroxamic acid. In the present context, it is to be understood that the invention also relates to specific regions of said inhibitors, that have never been specifically disclosed for the present purpose, as well as novel inhibitors identified by aid of the present invention. In specific embodiments, the complex according to the invention is composed of LTA4 hydrolase complexed with bestatin, thiolamine or hydroxamic acid, respectively, wherein the LTA₄ hydrolase is as defined by the coordinates presented in Table 9, or any functional fragment, derivative or analogue thereof. As bestatin is aminopeptidase based, further similar and advantageous inhibitors may be developped based on the structural information for LTA₄ hydrolase complexed with bestatin, preferably combined with the specification of the binding site of Table 2. Further, as both thiolamine is leukotriene based, the information provided in Table 9, preferably combined with the specification of binding site of Table 3, will prove to be an advantageous tool in order to gain more information about such enzymatic binding and thus the development of further

novel inhibitors, the same principles applying to hydroxamic acid, which is also leukotriene based.

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Accordingly, the present invention presents for the first time the coordinates defining the three-dimensional structure of a complex of LTA₄ hydrolase and an inhibitor thereof as determined by X-ray crystallography, e.g. as illustrated in Table 9. In fact, this is the first time ever to disclose the exact parameters defining the three-dimensional structure of a protein component of the leukotriene cascade. Due to these novel reliable parameters, the complex as well as the components thereof are readily distinguished from the prior art. Together with biochemical and mutagenetic data, the novel structures will provide the basis for understanding the molecular mechanisms of the aminopeptidase and epoxide hydrolase activities, as well as the enzyme's suicide inhibition. Accordingly, the present invention will open a whole range of new possibilities as regards e.g. identification and/or design of novel biologically active molecules and methods of controlling said cascade, *in vivo* or *in vitro*. Consequently, novel advantageous drugs, such as medicaments for the treatment

In the present context, it is to be understood that proteins according to the invention include the naturally occurring three dimensional forms thereof, separated and isolated from its natural environments, as well as any such protein, wherein deletions, additions and/or substitutions of the amino acid sequence have been made, provided that the three dimensional structure is substantially maintained, as the exerted biological activity is critically dependent upon the particular three-dimensional folding of the protein. The present invention also encompasses any derivative or conformational analogue of the above disclosed proteins, which has a three-dimensional structure essentially as disclosed above, or an effective part thereof having the biological activities discussed in detail below.

and/or prevention of inflammatory and/or allergic diseases, may be designed, as will

be discussed in further detail below.

2.4.4 Advantageous uses of LTA₄ hydrolase, complementary compounds and complexes thereof

A fourth aspect of the present invention is the use of a protein, a complementary compound or a complex according to to the invention in drug design, such as in molecular modeling, direct structure-based design and/or combinatorial chemistry. Such methods will be disclosed in detail below. The drugs designed using the above mentioned compounds may be suitable for the treatment and/or prevention of disorders involving acute and chronic inflammatory symtoms, said disorder being selected from the group consisting of arthritis, inflammatory bowel disease (IBD), psoriasis, chronic obstructive pulmonary disease (COPD), and acquired immune deficiency syndrome (AIDS). Further, such a drug may be useed for the treatment and/or prevention of proliferative disorders, such as neoplasias and/or cancer. Alternatively, a drug may be designed which is effective for the treatment and/or prevention of an inflammatory and/or allergic disorders caused by the lethal factor of Bacillus anthracis, e.g. anthrax. However, the above mentioned diseases are exemplary and other diseases or conditions not mentioned herein may also be contemplated.

In a further aspect, the present invention relates to the use of a protein having a structure substantially as defined for the LTA₄ hydrolase of the invention, or a part, analogue or derivative thereof, for screening a compound for possible medicinal activity. In the pharmaceutical industry, new or known compounds are routinely screened for new uses employing a variety of known *in vitro* or *in vivo* screens. Often such screens involve complex natural substances and are consequently expensive to carry out, and the results may be difficult to interpret. However, the knowledge of the three-dimensional protein structure according to the invention allows a preliminary screening to be carried out on the basis of the three-dimensional structure of a region thereof, and the structural similarity of a molecule which is being screened. Such screening can conveniently be carried out using computer modelling techniques, which match the three-dimensional structure of the protein or part thereof with the structure of the molecule being screened. Potential agonist or inhibitor activity may be predicted. As a result, the production efficiency, bioavail-

ability, immunogenicity, stability etc. may be favourably changed with respect to their therapeutic application.

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As regards the above disclosed M1 inhibitors, these compounds will presumably find a broader field of application than the other novel inhibitors according to the invention. Thus, the novel general M1 inhibitors are advantageously used e.g. in models to disclose in further detail other enzymatic pathways. Further, they may also be used in the above mentioned type of methods of drug design etc.

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2.4.5 Screening for LTA₄ hydrolase analogues

2.4.5 (a) Method

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Accordingly, in another aspect, the invention relates to a method for screening LTA₄ hydrolase analogues that mimic at least a part of the three dimensional structure of LTA₄ hydrolase, which comprises the steps of

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(a) producing a multiplicity of analogue structures of the LTA₄ hydrolase

(b) selecting an analogue structure represented by a three-dimensional representation wherein the three-dimensional configuration and spatial arrangement of specific regions, preferably involved in ligand binding of said LTA4 hydrolase, remain substantially preserved.

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The coordinates used are general for LTA₄ hydrolase are essentially as illustrated in Table 9, as defined by atom nos. 1-4876.

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More specifically, analogue structures of LTA4 hydrolase may be screened by their ability to catalyze a particular reaction which may be monitored by chemical physical or immunological means. Furthermore, the analogue structure may be selected from its ability to produce receptor ligands or inhibitors of secondary reactions, which may be monitored directly, as examplified above, via binding assays,

25 enzyme assays, chemical assays, or functional bioassays.

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Thus, in one embodiment, the invention relates to a method of screening. wherein one or more analogues exhibiting epoxide hydrolase activity, are screened for. Thus, such a method may be based on the data of Table 9, wherein the binding of thiolamine to LTA₄ hydrolase is shown, preferably combined with the information of Table 3 regarding the active site of LTA₄ hydrolase. In one embodiment, the

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invention relates to a method of screening, wherein one or more analogues exhibiting epoxide hydrolase activity, are screened for. In an alternative embodiment, the present method is used to screen for analogues exhibiting aminopeptidase activity, which method e.g. is based data concerning the binding of bestatin to LTA₄ hydrolase is used, preferably combined with the information of Table 2 regarding the active site of LTA₄ hydrolase. Thus, the present analogues will comprise a region which is essentially analogue with the regions of LTA₄ hydrolase exhibiting aminopeptidase activity, and/or analogues exhibiting epoxide hydrolase activity are selected.

In an advantageous embodiment of the screening method according to the invention, one or more analogues comprising one or more genetic modifications, as compared to the naturally occurring form of LTA₄ hydrolase, are selected.

2.4.5 (b) Analogues obtainable by the present screening method

Further, the invention also relates to a novel analogue obtainable by the method according to the invention, such as an analogue exhibiting an increased or improved or otherwise modified catalytic activity when compared to the naturally occurring form of LTA₄ hydrolase. Preferably, said catalytic activity is an epoxide hydrolase and/or aminopeptidase activity. Further, the invention relates to an analogue obtainable by the present method and capable of acting as a metallohydrolase, preferably belonging to the M1 class of metallohydrolases.

2.4.5 (c) Mutated forms of LTA₄ hydrolase obtainable by the present screening method

In one advantageous embodiment, the present invention relates to a specified analogue which is a mutated form of LTA₄ hydrolase, which analogue comprises one or more of the mutations defined in the following Tables 5-7, wherein amino acids are given in single letter code. Thus,

Q134G/A/V/L/I/S/T/D/E/N/R/H/K/P/C/M/F/Y/W indicates that residue glutamine 134, using the LTA4 hydrolase numbering scheme, is modified to an alanine, valine, a leucine and so forth.

5 Table 5: Mutations in the active site O134G/A/V/L/I/S/T/D/E/N/R/H/K/P/C/M/F/Y/W 5(1) Q136G/A/V/L/I/S/T/D/E/N/R/H/K/P/C/M/F/Y/W 5(2) 5 A137G/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W 5(3) 10 Y267G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/W 5(4) G268A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W 5(5) G269A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W 56) M270G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/F/Y/W 5(7) 10 E271G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W 5(8) 15 V292G/A/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W 5(9) H295/G/A/V/L/I/S/T/D/E/N/Q/R/K/P/C/M/F/Y/W 5(10) E296/G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W 5(11) H299G/A/V/L/L/S/T/D/E/N/Q/R/K/P/C/M/F/Y/W 5(12) 15 W311G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y 5(13)20 F314G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/Y/W 5(14) W315G/A/V/L/I/S/T/D/E/N/O/R/H/K/P/C/M/F/Y 5(15) E318G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W 5(16) V322G/A/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W 5(17) F362G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/Y/W 20 5(18) 25 V367G/A/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W 5(19)L369G/A/V/I/S/T/D/E/N/O/R/H/K/P/C/M/F/Y/W 5(20) 1372G/A/V/L/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W 5(21) P374G/A/V/L/I/S/T/D/E/N/Q/R/H/K/C/M/F/Y/W 5(22) 25 D375G/A/V/L/I/S/T/E/N/Q/R/H/K/P/C/M/F/Y/W 30 5(23) A377G/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/Y/W 5(24) Y378G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/W 5(25) P382G/A/V/L/I/S/T/D/E/N/Q/R/H/K/C/M/F/Y/W 5(26)Y383G/A/V/L/I/S/T/D/E/N/Q/R/H/K/P/C/M/F/W 5(27) 35 R563G/A/V/L/I/S/T/D/E/N/Q/H/K/P/C/M/F/Y/W 30 5(28) More specifically, this embodiment relates to an analogue comprising any combination of at least two mutated amino acids, or any one of the above mentioned sequen-40 ces of mutations, or any separate one amino acid mutation selected from the group 35 consisting of sequences nos 1-9, 13-15, 17-24, 26 and 28, which are all novel mutations that have never been published before the present application. As two specific 45 embodiments of the present mutations according to the invention, E271Q and D375N are mentioned, which have shown to be especially advantageous. However, the other sequences not specified above are novel in the present context and thus 40 such specific uses thereof are within the scope of the present invention.

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5		Table 6: Mutations of the curved outside of the N-to	erminal domain
		R17 G/A/V/L/I/S/T/D/N/E/Q/H/K/P/C/M/F/Y/W	6(1)
		K19 G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W	6(2)
		H20 G/A/V/L/I/S/T/D/N/E/Q/R/K/P/C/M/F/Y/W	6(3)
	5	H22 G/A/V/L/I/S/T/D/N/E/Q/R/K/P/C/M/F/Y/W	6(4)
10		R24 G/A/V/L/I/S/T/D/N/E/Q/H/K/P/C/M/F/Y/W	6(5)
		D28 G/A/V/L/I/S/T/N/E/Q/R/H/K/P/C/M/F/Y/W	6(6)
		T33 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(7)
		T35 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(8)
	10	G36/A/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(9)
15		T37 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(10)
		A39 G/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(11)
		T41 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(12)
		Q43 G/A/V/L/I/S/T/D/N/E/R/H/K/P/C/M/F/Y/W	6(13)
20	15	K63 G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W	6(14)
20		V65 G/A/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(15)
		N67 G/A/V/L/I/S/T/D/E/Q/R/H/K/P/C/M/F/Y/W	6(16)
		N97 G/A/V/L/I/S/T/D/E/Q/R/H/K/P/C/M/F/Y/W	6(17)
		E99 G/A/V/L/J/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	6(18)
25	20	V101 G/A/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(19)
25		E103 G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	6(20)
		S105 G/A/V/L/I/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(21)
		E107 G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	6(22)
		K153 G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W	6(23)
30	25	T155 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(24)
		T157 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(25)
		E159 G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	6(26)
		\$161 G/A/V/L/I/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(27)
		D175 G/A/V/L/I/S/T/N/E/Q/R/H/K/P/C/M/F/Y/W	6(28)
35	30	E177 G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	6(29)
		T178 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(30)
		D180 G/A/V/L/I/S/T/N/E/Q/R/H/K/P/C/M/F/Y/W	6(31)
		R186 G/A/V/L/I/S/T/D/N/E/Q/H/K/P/C/M/F/Y/W	6(32)
		I188 G/A/V/L/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(33)
40	35	K190 G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W	6(34)
	33	I192 G/A/V/L/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	6(35)
		K194 G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W	6(36)
			0(30)
45		Table 7: Mutations at the proline rich re	gion
	40	T359 G/A/V/L/I/S/D/N/E/Q/R/H/K/P/C/M/F/Y/W	7(1)
		E358 G/A/V/L/I/S/T/D/N/Q/R/H/K/P/C/M/F/Y/W	7(2)
		D443 G/A/V/L/I/S/T/N/E/Q/R/H/K/P/C/M/F/Y/W	7(3)
50		A446 G/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	7(4)
		Y449 G/A/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/W	7(5)
	45	S450 G/A/V/L/I/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	7(6)

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5		P451 G/A/V/L/I/S/T/D/N/E/Q/R/H/K/C/M/F/Y/W	7(7)
		G452 /A/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	7(8)
		L453 G/A/V/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	7(9)
		P454 G/A/V/L/I/S/T/D/N/E/Q/R/H/K/C/M/F/Y/W	7(10)
40	5	P455 G/A/V/L/I/S/T/D/N/E/Q/R/H/K/C/M/F/Y/W	7(11)
10		I456 G/A/V/L/S/T/D/N/E/Q/R/H/K/P/C/M/F/Y/W	7(12)
		K457 G/A/V/L/I/S/T/D/N/E/Q/R/H/P/C/M/F/Y/W	7(13)
		P458 G/A/V/L/I/S/T/D/N/E/Q/R/H/K/C/M/F/Y/W	7(14)
		N459 G/A/V/L/I/S/T/D/E/Q/R/H/K/P/C/M/F/Y/W	7(15)
15	10	Y460 G/A/V/L/I/S/T/D/N/E/Q/R/H/K/P/C/M/F/W	7(16)
, ,		D461 G/A/V/L/I/S/T/N/E/Q/R/H/K/P/C/M/F/Y/W	7(17)

2.4.5 (d) Nucleic acids encoding the novel compounds

Further, the invention also relates to an isolated nucleic acid encoding a novel analogue as defined above, that is, including a combination of any at least two of said mutations or one of the novel mutations, as well as a nucleic acid capable of specifically hybridising to a such a nucleic acid. The conditions of specific hybridisation are defined above in the section "Definitions". Further, the invention also relates to any vector or carrier comprising such a nucleotide, such as plasmids, viral vectors, e.g. retrovirus, oligonucleotides etc. Thus, any cell including such a nucleic acid or vector are also within the scope of the present invention and may e.g. be a mammalian cell, such as a human cell, or any other eucaryotic cell, or a procaryotic cell, such as a bacterium. The above mentioned elements may be used in the design of model systems useful in the study of the diseases discussed elsewhere in this application, which systems may be cell cultures, animal models, such as mice, etc.

2.4.6 (a) Production and purification of genetically modified forms of LTA₄ hydro-

Yet another aspect of the present invention is a process for the production of a novel genetically modified form of LTA₄ hydrolase identified or designed according to the present invention. Thus, the present process involves, after conventional steps of insertion a gene encoding the desired product in a host cell and expression thereof, a purification procedure, which includes a hydroxyapatite-based chromatography and a subsequent anion exchange chromatography. These last two steps have been shown to be especially advantageous, in fact, even crucial, for obtaining a

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satisfying purity of the novel LTA₄ hydrolase forms according to the invention. The preceding steps are conventional as disclosed in literature and are easily performed by the skilled in this field.

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Thus, in more detail, the invention relates to a method for purification of LTA4 hydrolase comprised of (i) precipitation with ammonium sulphate, followed by (ii) separations on FPLC using anion exchange, hydrophobic interaction, and chromatofocusing resins, essentially as described (Wetterholm A., Medina J.F., Rådmark O., Shapiro R., Haeggström J.Z., Vallee B.L., Samuelsson B. *Biochim. Biophys. Acta.* 1080, 96-102 (1991)). To achieve a purity suitable for crystallography, we used (iii) chromatography on hydroxyapatite, e.g., on a TSKgel HA-1000, Tosohaas, followed by (iv) a step of anion-exchange chromatography on e.g., Mono-Q HR5/5.

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Further, example 4 below describes in detail a purification of LTA₄ hydrolase according to the invention. Said example may be generalised to describe further the purification according to the invention.

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15 2.4.6 (b) Purified LTA₄ hydrolase

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Further, the invention also relates to an essentially pure form of LTA₄ hydrolase obtained by the process described above.

2.4.7 (a) Method

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In yet a further aspect, the present invention relates to a method for screening LTA₄ hydrolase binding compounds complementary to a region, preferably an enzymatically active site, e.g. as defined in Tables 1-3, of the LTA₄ hydrolase molecule, which comprises the steps of

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(a) producing a multiplicity of possible complementary structures and

2.4.7 Identification of LTA₄ hydrolase binding compounds

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(b) selecting a structure represented by a three-dimensional representation, wherein the three-dimensional configuration and spatial arrangement of regions of LTA₄ hydrolase involved in binding remain substantially preserved, which selection is based on the three-dimensional structure of LTA₄ hydrolase and/or LTA₄ hydrolase complexed to an inhibitor thereof, e.g. as defined by the coordinates of Table

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More specifically, the method according to the invention will advantageously be used to select compounds capable of inhibiting epoxide hydrolase activity and/or aminopeptidase activity, LTB₄ receptor antagonists or inhibitors of LTC₄ synthases or inhibitors of any member of the M1 class of metallohydrolases. In one preferred embodiment, general enzyme inhibitors are screened for, which inhibitors are useful in the control of any one of a plurality of enzymatic pathways, wherein a metallohydrolase of the M1 type is participating. These general metallohydrolase inhibitors are herein denoted M1 inhibitors.

Structure-based design of inhibitors

In a further embodiment, the present invention relates to a method of structure-based design of LTA₄ hydrolase inhibitors. Such methods are based on the use of the present coordinates, or preferably the coordinates defining a selected region, as templates in order to synthesize advantageous inhibitors with strong and specific binding properties. More specifically, said method first uses a conventional organic synthesis, alone or combined with combinatorial chemistry, wherein the structure of the product of the synthesis is then further refined by cycles of crystallisation of enzyme and inhibitor, followed by another chemical synthesis, the product of which is again refined, etc.

Example 2 describes such a design, wherein it is noted noted that the removal of an extra carbon atom could yield a compound, which is a better inhibitor than this hydroxamic acid compound. Thus, similar conclusions will be drawn from the present method and result in inhibitors with superior properties compared to any prior art inhibitors.

2.4.7 (b) Identified binding compounds

Further, the present invention also relates to any novel compounds identifiable by the present method. Advantageous and desired properties as well as other features of such compounds, e.g. as inhibitors, is discussed above in relation to complementary compounds, analogues etc. In one preferred embodiment of the invention, such an identified compound is an inhibitor of another M1 enzyme than LTA₄ hydrolase, such as . The medicinal aspects of the present compounds will be discussed below.

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Protein engineering

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2.4.8 (a) Method

In a further aspect, the present invention relates to a method of engineering a protein, which method comprises the steps of

-identification of a suitable set of mutation sites based on the structure of LTA₄ hydrolase according to the invention,

-generation of a library of genes which contains the suitable sequence variations;

-selection of clones encoding a LTA₄ analogue with a desired activity; wherein said desired activity is the capability of efficiently producing organic compounds of interest.

The present method is based on recent techniques available for generating large libraries of mutated genes (>1 billion variants) which can be attributed to a selection process of individual genes in the laboratory. Such directed evolution schemes have enormous potential for the design of new proteins, including new substrate specificity for enzymes as well as improving enzyme activities.

Directed evolution, or combinatorial engineering schemes have been successfully applied in evolving RNA molecules with improved binding and catalytic activities (Lorsch and Szostak, 1994). Also binding proteins (and peptides) with good affinities can now routinely be evolved based on a range of different protein folds (Nord et al, 1997). The present methods may be used to perform such a directed evolution of advantageous enzyme activity and specificity and may be performed by someone skilled in this field with reference to the literature, see e.g. O. Kuchner and F. H. Arnold (1997); A. Crameri, S.A. Raillard, E. Bermudez and W.P.C.

Stemmer (1998).) In this context, see also the descriptions provided in US patent no 5 873 082, Noguchi, wherein a list processing system for managing and processing lists of data is disclosed; US patent no 5 869 295, LaBean et al., disclosing methods and materials for producing gene libraries; and US patent no 5 856 928, disclosing a process for gene and protein representation, characterization and interpretation thereof.

In general, major difficulties in this kind of process are to search the sequence space: find the suitable sequence variations for a large but limited number of muta-

tions (for the same protein fold an immense number of variations can be made e.g. 10 resides protein, 20^{100} variants are in theory possible). It is therefor very important to identify the residues in the protein structure which could effect the activity the most, i.e. the residues near the active site area. Thus, in order to enable a successful performance of a method for engineering proteins with properties relevant in the present field, the data discosed above, more specifically, in Tables 2-4, is crucial.

Further references which are relevent in the context of protein engineering are K. Nord, E. Gunneriusson, J. Ringdahl, S. Stahl, M. Uhlen, P.A. Nygren (1997): "Binding proteins selected from combinatorial libraries of an alpha-helical bacterial receptor domain", *Nature Biotechnology*, 15, 772-777 (1997); R. Lorsch and J.W. Szostak (1994): "In vitro evolution of new ribozymes with polynucleotide kinase activity", *Nature*, 371, 31-36; A. Crameri, S.A. Raillard, E. Bermudez and W.P.C. Stemmer (1998): "DNA shuffling of a family of genes from diverse species accelerates directed evolution", *Nature*, 391, 288-291; and O. Kuchner and F. H. Arnold (1997): "Directed evolution of enzyme catalysts", *Trends in Biotechnology*, 15, 523-530.

In an advantageous embodiment, the present method is used to engineer LTA₄ hydrolase inhibitors and/or analogues. In a specific embodiment of said method, a compound capable of mimicking the suicidal mode of LTA₄ hydrolase catalysis, thus acting as a mechanism-based suicide inhibitor, or otherwise capable of regulating the production of LTB₄ is engineered. In an alternative embodiment, an inhibitor of LTC₄ synthase or an LTB₄ receptor antagonist is designed.

2.4.8 (b) Novel specifically designed proteins

Further, the present invention also relates to any novel protein designed by use of the above described method. Once specified, such proteins may be produced by any conventional method well known to the skilled in this field, some of which are examplified below. In Example 2 below, the binding of hydroxamic acid to LTA4 hydrolase is discussed. Thus, such a modified hydroxamic is one example of a novel inhibitor specifically designed according to the invention, and the resoning in the

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example may be used as a basis for the way of reasoning that is used in the present design.

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Accordingly, novel enzymes may be produced, which are capable of any different chemical activity. For example, enzymes capable of novel catalytic properties, enzymes that in turn produce enzymes, etc., may be produced according to the present invention.

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2.4.8 (c) Use of genetically modified LTA₄ hydrolase

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The invention also encompasses the use of a genetically modified LTA4 hydrolase, obtained by any method according to the invention, with altered catalytic properties, e.g., increased ability to synthesize LTB4. The modified enzyme may thus be used for production of LTB4, or any analogues substances, a biomedical reagent which in turn may be used in, e.g., studies of leukotriene metabolism, induction of chemotaxis, as a reference compound in analysis of leukotrienes etc.

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2.4.9 Pharmaceutical applications of the present invention

15 2.4.9 (a) First medical indication

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Further, the invention also encompasses a compound obtainable by the method of screening LTA₄ hydrolase binding compounds, structure-based drug design, or the protein engineering methods described above, and more preferably, said compound for use as a medicament. One specifically advantageous embodiment is the herein disclosed novel M1 inhibitor for use as a medicament.

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In an advantageous embodiment, the present compounds are used in the manufacture of a medicament for the treatment and/or prevention of acute and chronic inflammatory disorders, said disorder being selected from the group consisting of arthritis, inflammatory bowel disease (IBD), psoriasis and chronic obstructive pulmonary disease (COPD); neoplasias and/or cancer; or disorders caused by the lethal factor of *Bacillus anthracis*, e.g. anthrax. Alternatively, the use may relate to the manufacture of a medicament for the treatment and/or prevention of an inflammatory and/or allergenic disorder, such as bronchial asthma, allergic rhinitis, conjunctivitis etc. Yet an alternative use is in the manufacture of a medicament for the treatment and/or prevention of infection caused be human immunodeficiency virus

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(HIV). The novel M1 inhibitor are preferably used in medicaments for the treatment and/or prevention of such various diseases as cancer and/or endochrinological disturbances.

2.4.9 (b) Second medical indication and pharmaceutical methods

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Thus, the present invention relates to the above mentioned molecules prepared by the method according to the invention for use in the manufacture of various medicaments for the above defined conditions. The invention also encompasses pharmaceutical preparations containing these molecules together with pharmaceutically acceptable carriers. Methods for the preparation of pharmaceutical preparations are e.g. found in Remington's Pharmaceutical Sciences, Mack Publishing Company, Philadelphia, PA, 17th ed. (1985). For a review of drug delivery, see Langer, Science 249:1527-1533 (1990). As those skilled in this field easily realise, the form of

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2.4.9 c) Methods of treatment

The present invention also encompasses any method of treatment for the above defined purposes. Exact details regarding such methods are determined by the practitioner depending on the specific circumstances from case to case.

such a pharmaceutical preparation, the mode of administration thereof as well as

suitable dosages will depend on the specific disease to be treated, the nature of the

2.5 Production of novel proteinaeous compounds

active substance used, the patient's age, body weight etc.

The compounds, which may be proteins, polypeptides, peptides or any other organic molecules, prepared according to the methods according to the invention may be synthesized chemically by methods well known to those of skill in this field or they may be prepared by use of recombinant DNA technology by any suitable method well known to those of skill in this field. General methods of synthesis are e.g. found in Berger and Kimmel, Guide to Molecular Cloning Techniques, Methods in Enzymology, vol. 152, Academic Press, Inc., San Diego, CA; Sambrook et al., Molecular Cloning, A Laboratory Manual, 2nd Ed., vol. 1-3, Cold Spring Harbor Laboratory, Cold Spring Harbor, NY, 1989; and Current Protocols in Molecular Biology, F.M. Ausbel et al., Current Protocols (1994). Methods of reducing and denaturing proteins and inducing re-folding are well known to those of skill in the art,

see e.g. Debinski et al., J. Biol. Chem., 268: 14065-14070 (1993); Kreitman and Pastan, Bioconjug. Chem., 4: 581-585 (1993); and Buchner et al., Anal. Biochem., 205: 263-270 (1992).

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2. 6 Detailed description of the drawings

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Figure 1 shows key enzymes and intermediates in leukotriene biosynthesis.

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Figure 2 shows 2Fo-Fc density contoured at 1.1 σ . Part of the active site in the neighborhood of the bestatin molecules is shown. Figures are created using a modified

version of Molscript48,49.

Figure 3 is a ribbon diagram of the tertiary structure of LTA4 hydrolase. The N-

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terminal domain at the top of the diagram is rich in \beta-strands and connects to the catalytic domain to the left in the figure which is more \alpha-helical and extends into

the central part of the molecule. The C-terminal domain, illustrated at the bottom of

the ribbon diagram, extends towards the right side of the catalytic domain.

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Figure 4 (a) is a ribbon diagram of the N-terminal domain with its layers of β-

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strands, while (b) is a superimposition of the $C\alpha$ trace of the N-terminal domain on the Ca trace of bacteriochlorophyll a. The N-terminal domain covers approx. half of

the bacteriochlorophyll a structure (the right and bottom part of the diagram).

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Figure 5 (a) is a ribbon diagram of the catalytic domain. In the center of the dia-

gram, the three zinc binding ligands, His295, His299, and Glu318, as well as the in-

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as a CPK model. The diagram in (b) shows the structure of thermolysin in the same

orientation as the catalytic domain of LTA4 hydrolase. The three zinc ligands,

His142, His146, and Glu166, as well as the inhibitor Cbz-GlyP-(O)-Leu-Leu50 are

depicted in ball-and stick representation. The zinc ion is shown as a CPK model.

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25 Figure 6 shows the structure of the C-terminal domain.

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Figure 7 shows the zinc binding ligands in LTA4 hydrolase, His295, His299, and Glu318, superimposed on those in thermolysin, His142, His146, and Glu-166. Other catalytic or neighboring residues in the two enzymes are Tyr383, Glu325, Glu296,

Thr302, and Asn317 in LTA4 hydrolase which correspond to His231, Asp170,

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Glu143, Asn165, and Tyr157 in thermolysin.

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Figure 8 (a) is a Ball-and-Stick presentation of the binding of bestatin in LTA4 hydrolase.

Figure 8 (b) is a schematic overview of bestatin binding in LTA4 hydrolase.

Figure 9 (a) is a wire representation of the cavity found in LTA4 hydrolase (shown as Cα-trace).

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as Cα-trace).

Figure 9 (b) is a schematic presentation for the proposed binding of LTA4 into the

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Figure 9 (b) is a schematic presentation for the proposed binding of LTA4 into the cavity.

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Figure 10 is a schematic representation for the proposed epoxide hydrolase reaction mechanism. The catalytic zinc acts as a Lewis acid and activates the epoxide to form a carbocation intermediate according to an S_{N1} reaction. Water is added at C12 in a stereospecific manner, presumably directed by Asp375. The double bond geometry is controlled by the binding conformation of LTA4. Further details are given elsewhere in the present description.

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15 <u>3. EXPERIMENTAL</u>

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The following examples are intended for illustrating purposes only and should not in any way be used to construe the scope of the protection of the present invention as defined by the appended claims. All the references given below, and previously in this specification, are hereby included herein by reference.

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3.1 Examples

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Example 1: Binding of the thiol-compound (I)

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The thiol group of the compound is ligated to the Zn²⁺ ion, that has a tetra-hedral configuration. Both the phenyl-groups are making extensive hydrophobic interactions. The first one makes aromatic stacking interactions with Phe314 and Trp311. Further hydrophobic interactions are made with Pro374 and Leu369. The other phenyl ring is making stacking interactions with Tyr267 and Tyr378. Met270 and Gln136 provide additional hydrophobic interactions. The ether-oxygen in the linker between the two phenyl rings makes a hydrogen bond to the backbone nitrogen of

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Ala137 and also with a water molecule which is linked to Asp375. The amine group makes interactions to the OE1 of Gln136 and the OE1 of Glu271.

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5 Formula (I)

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Oel Gln136 O∈1 Glu271 Trp311 Phe314 Тут267 Met270 Gln136 Leu369 2.1 Tyr378 Pro374 N Ala137 Phe314 1.9 Oδ1 Asp375 O∈1Glu 318

Example 2: Binding of the hydroxamic acid compound (II)

The binding of this compound is very similar to the binding of the thiol compound described above. The manner in which the phenyl-moieties, the linker region and the amine group are bound is identical. The manner in which the hydroxamic acid part is bound is different in comparison with other complexes such as thermolysin-HA complexes and LTA₄-hydrolase-bestatin complex. Instead of a double interaction of the hydroxyl and carbonyl oxygens and the Zn ion resulting in a pentavalent co-ordination, here only one of the oxygens (the hydroxyl) is making an interaction with the Zn ion giving a tetrahedral co-ordination. The other oxygens make an interaction to Asp296 and the backbone nitrogen of Gly268. This difference is probably due to the tight binding of the phenyl rings and the amine group. The linkage between the amine group and the hydroxamic acid group contains one more carbon atom than in a normal or modified peptide-linkage. Since the binding site for substrates is rather narrow near the Zn ion, the conformation of compounds which bind in this area is rather restricted. Therefore one of the otherwise binding oxygens is pushed out and can no longer make an interaction with the Zn²⁺ ion. Removal of this extra

carbon atom could yield a compound which is a better inhibitor than this hydroxamic acid compound. The acid group at the other end of the compound is fixed by making a double interaction with the NE and the Nh2 of Arg563.

Oct Gln136

Тут383

Gly268

N Gly268

Gly269

Nh2 Arg56

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Os1 Glu271 Trp311 Phc314 Tyr267 15 Met270 Gln136 Leu369 Pro374 Phe314 20

N Ala137

Oδ1 Asp375

Formula (II)

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Example 3: Structure determination of two specific inhibitor-LTA₄ hydrolase complexes

Oδ1 Ghi296

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Crystals, grown as described above, were soaked in 1 mM solution of thiolamine (Yuan et al., 1993) or 0.5 mM solution of hydroxamic acid (Hogg et al., 1995) in 15% PEG8000, 50 mM Imidazol pH 6.7, 25 mM acetate and 2.5 mM YbCl3. After at least 24 hours, the crystals were transferred to a solution that contained a cryoprotectant (see above) and subsequently flash frozen in liquid nitrogen. The data for the crystal soaked with thiolamine was obtained at BM14B at the EMBL-outstation in DESY, Hamburg. The data for the hydroxamic acid was collected at beamline 7/11 at MAX-lab, Lund. Statistics from the data collections are shown in the table. The data were processed using MOSFLM, merging and other manipulations were performed by programs from CCP4 and the BIOMOL packages. The refinement procedures for both datasets were very similar. First rigid body refinement using TNT was performed. As a starting model for refinement and model building the structure of LTA4 hydrolase complexed with bestatin was used. The bestatin molecule and all water molecules were deleted from the model. After this initial refine-

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ment it was possible to build the inhibitors into the protein. For evaluation of the density maps and model-building the program QUANTA (Molecular Simulations Inc., Burlington, MA) was used. The refinement was continued using TNT and was combined with sessions of model-building. In all rounds no sigma cut-offs were used and the resolution was slowly increased during the procedure. Water molecules were identified and incorporated into the models. During these procedures the Rfree was carefully monitored. When refinement had converged, it was finished with one round in which all reflections, including those who were used for the calculations of the Rfree, were incorporated. Statistics about refinement and quality of the models can be found in Table 5.

Table 8: Statistics of refinement and quality of the model

	Thiolamine (Thiol)	Hydroxamic acid (HA)
Resolution	15-2.5Å	15-1.8Å
Rfactor	17.8%	24.2%
Rfree	24.4	29.7%
Bond Lengths	0.011Å	0.012Å
Angles	1.9°	2.0°
Trigonal groups	0.005Å	0.006Å
Planar groups	0.009Å	0.010Å
Contacts	0.026Å	0.041Å
No. of waters	252	127

Example 4: Purification of LTA4 hydrolase.

For adsorption chromatography on hydroxyapatite, a TSKgel HA-1000 column (Tosohaas) was equilibrated in 10 mM potassium phosphate buffer, pH 7.1, supplemented with 0.2 mM CaCl₂. The enzyme sample was applied and a linear gradient of increasing phosphate (10 - 400 mM) was developed by mixing the starting buffer with 400 mM potassium phosphate buffer, pH 6.8, supplemented with 10 μ M CaCl₂. Active fractions containing LTA4 hydrolase were eluted between 150 - 190 mM potassium phosphate.

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Anion exchange chromatography was performed on a Mono-Q HR 5/5 column (Pharmacia Biotech) equilibrated with the loading buffer 10 mM Tris-Cl, pH 8. The pure protein was eluted using a linear gradient of KCl (0 - 500 mM) and was recovered at 110 - 140 mM KCl.

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Example 5: Enzyme engineering

The present inventors have shown, that when Tyr-378 in LTA4 hydrolase was exchanged for a Phe residue, the resulting mutated enzyme was no longer suicide inhibited by LTA4 and exhibited a substantially increased catalytic efficiency. Furthermore, the mutated enzyme was capable of converting LTA4 not only into the natural product LTB4, but also into a novel metabolite, 6-trans-8-cis-LTB4. (Mueller, M.J., et al. Proc Natl Acad Sci U S A 93, 5931-5935 (1996)).

Example 6: Enzyme-engineering

Tyr-383 in mouse LTA4 hydrolase was exchanged for Gln residue, which resulted in a mutated enzyme capable of forming the unnatural product 5S, 6S-dihydroxy-7,9-trans-11,14-cis-eicosatetraenoic acid from LTA4 (Andberg, M., Hamberg, M. & Haeggstrom, J.Z. J. Biol. Chem. 272, 23057-23063 (1997)).

Example 7: Crystallisation of LTA₄ hydrolase

LTA₄ hydrolase was crystallised using YbCl₃ as an additive, 15% PEG and 50 mM Na-acetate as precipitant and 50 mM imidazole, pH 6.7, as buffer. Liquid-liquid-diffusion in capillaries were used as crystallisation set-ups.

3.2 Materials and Methods

Enzyme purification. Human recombinant LTA4 hydrolase was expressed in E. coli and purified to homogeneity in four chromatographic steps on FPLC using anion exchange, hydrophobic interaction, chromatofocusing, and hydroxyapatite resins, essentially as described (Wetterholm A., Medina J.F., Rådmark O., Shapiro R., Haeggström J.Z., Vallee B.L., Samuelsson B. Recombinant mouse leukotriene A4 hyd-

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rolase: a zinc metalloenzyme with dual enzymatic activities. *Biochim. Biophys. Acta.* 1080, 96-102 (1991)).

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Crystallization conditions. The chemicals used for the crystallization experiments were purchased from Merck and were of highest purity available. The sparse matrix kit was obtained from Hampton Research. Crystallization conditions for the protein were initially sought by using the sparse matrix approach (Jancarik, J. & Kim, S.-H. J. Appl. Crystallogr. 24, 409-411 (1991)) in hanging drop vapor diffusion set-ups in cell culture plates at room temperature. Under condition 28, (30% PEG8000, 0.2 M sodium-acetate, 0.1 M cacodylate buffer, pH 6.5) needles grew. They were subsequently reproduced and optimized using a finer grid search, different temperatures for the equilibration and testing of additives. Crystals were only obtained when the inhibitor bestatin was present in the crystallization set-ups. Using YbCl3 as an additive and switching to liquid-liquid diffusion in capillaries, allowed plate-like crystals to grow. Thus, 5 µl 28% PEG8000, 0.1 mM Na-acetate, 0.1 mM imidazole buffer, pH 6.8, 5 mM YbCl3 is injected into the bottom of a melting point capillary and an equal volume of LTA4 hydrolase (5 mg/ml) in 10 mM Tris-Cl, pH 8, supplemented with 1 mM bestatin, is layered on top. Finally, the capillary is closed and stored at 22°C. Crystals with an average size of 0.6 x 0.4 x 0.05 mm³ appear in 3 to 4 weeks.

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<u>Crystal properties</u>. The plate-like crystals diffract beyond 2Å using synchrotron radiation. They belong to space-group P21212 with cell dimensions a = 67.59 Å, b = 133.51 Å, c = 83.40 Å, $a = b = g = 90 ^{\circ}$ at 100K. As a cryo-solution, a mixture of 15%PEG 8000, 50 mM Na-acetate, 50 mM imidazole buffer, pH 6.8, 2.5 mM YbCl3, and 25% glycerol was used. Assuming one molecule per asymmetric unit the solvent content of the crystals is 48%.

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Structure determination. The structure was determined by using multiple anomalous dispersion measurements on the LIII edge of Ytterbium ($\lambda = 1.3862$ Å) at beam line BM14 at the European Synchrotron Radiation Facility (ESRF), Grenoble. Three datasets, peak (PK), point of inflection (PI) and remote (RM), were collected to 2.5Å resolution from the same crystal. The crystal was aligned such that Bijvoet

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equivalent reflections could be collected in one pass of 90° for each wavelength. For RM a subsequent dataset to 2.15Å was collected. A second crystal was used for obtaining a dataset to 1.95Å. (For statistics on data-collection and quality, see table 1). Data were integrated using the program Denzo, scaled to each other using Scalepack (Otwinowski, Z. Data collection and Processing. Proceedings of the ccp4 study weekend. SERC Daresbury Laboratory, Warrington, UK., 56-62 (1993)) and further analyzed using programs from the CCP4 package (Collaborative Computing Project Number 4. Acta Crystallogr. Sect. D 50, 760-763 (1994)).

From Patterson functions one major and one minor Yb position could readily be identified, a third position was identified during heavy atom refinement in difference Fourier maps. The heavy atom parameters were refined using MLPHARE (Otwinowski, Z. Isomorphous replacement anomalous scattering. Proceedings of the CCP4 study weekend. SERC Daresbury Laboratory, Warrington, UK., 80-85 (1991)) and SHARP (de La Fortelle, E. & Bricogne, G. Met. Enzymol. 276, 472-494 (1997)). The final figures of merit was 0.57 to 2.15Å. Phase information was further improved to 2.15Å by solvent flattening using SOLOMON (Abrahams, J.P. & Leslie, A.G.W. Acta Crystallographica D52, 30-42 (1996)) with a solvent content of 43%. The quality of the maps was very good and the entire protein molecule (residue 1-610) could be traced unambiguously. All model building was performed using QUANTA (Molecular simulations). Refinement was started by a run of slowcooling molecular dynamics in XPLOR (Brünger, A.T., Kuriyan, J. & Karplus, M. Science 235, 458-460 (1987)) using the RM dataset to 2.7Å. The three Yb ions were included into the refinement with full occupancy for the first Yb and half occupancy for the two other ions. All subsequent refinement was performed with TNT (Tronrud, D.E., ten Eyk, L.F. & Matthews, B.W. Acta Crystallogr. Sect. A 43, 481-501 (1987)). The same set of reflections (4% of total amount from 25-1.95Å) for the calculation of Rfee (Brünger, A.T. Nature 355, 472-475 (1992)) was maintained throughout all refinement procedures. The resolution was slowly improved by alternating sessions of model-building and refinement. The data for the second crystal to 1.95Å were used for further refinement during which a Zn ion, bestatin, an acetate

and an imidazole molecule were identified. Judged from the B-factors these molecules are all fully occupied. 540 water molecules were added to the coordinates. The Rfree was 24.7% and the working R-factor was 18.8% for all data between 25-1.95 Å. In a final round of refinement all data between 25-1.95 Å were included, yielding a final R-factor of 18.5 % for residues 1-610, 3 Yb ions, 1 Zn, 1 bestatin, 1 imidazole, 1 acetate and 540 water molecules. Most of the model is in good density (Fig. 2) except a loop encompassing residues 179 to 184 for which only poor density was obtained. The model has good stereo-chemical parameters (r.m.s bonds =0.010Å, r.m.s angles = 2.2°) and 91.7% of the residues lie in the most favored part of the Ramachandran plot.

4. RESULTS AND DISCUSSION

4.1 Overall structure and domain organization

The leukotriene A4 hydrolase molecule is folded into three domains; an N-terminal domain, a catalytic domain and a C-terminal domain which together form a flat triangular arrangement with approximate dimensions of $85 \times 65 \times 50 \text{ Å}^3$. The overall structure of the enzyme is depicted in figure 3. Although the three domains pack closely and make contact with each other, a deep cleft is formed in between.

4.2 The N-terminal domain is structurally related to bacteriochlorophyll a

The N-terminal domain (residue 1-209) is composed of one 7 stranded mixed b-sheet, one 4 and one 3 stranded antiparallel β -sheet. Strands from the larger β -sheet continue into the two smaller β -sheets that pack on the edges of the same side of the larger sheet so that a kind of envelope is formed (Fig. 4a & b). The two small β -sheets are turned towards the inside of the whole protein while the larger β -sheet is exposed to solvent and forms a large concave surface area. Loops connecting the other strands and hydrophobic residues fill the core of this domain. The N-terminal domain of LTA4 hydrolase shares important structural features with the chlorophyll-containing enzyme bacteriochlorophyll (Bchl) α (Matthews, B., Fenna, R., Bolognesi, M., Schmid, M. & Olson, J. J. Mol. Biol. 131, 259-285 (1979)). Thus, 111 C α positions have equivalent positions in the two proteins despite the absence

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of any sequence identity (Fig. 4b). The domain is about half the size of Bchl a which has a single domain structure without major extensions. Like Bchl a, the shape of the N-terminal domain resembles an envelope (or Taco) with a hollow inside and in Bchl a, 7 bacteriochlorophylls are buried in this cavity. However, the domain is not as hollow as BChl a since loop 135-155, which contains a small helical segment, is turned inwards and fills up the core. In BChl a the equivalent loop (290-305) is positioned more towards the exterior of the protein, thereby leaving space for some of the tertrapyrroles of the bacteriochlorophylls. The large sheet (17 strands) of Bchl a is truncated to only 7 strands in LTA4 hydrolase. Especially the region between residue 35 and 263 of Bchl a has been replaced by a much shorter region in LTA4 hydrolase (res. 45 to 98) that forms the 3 stranded small β-sheet and the edge strand of the larger 7 stranded β-sheet. The structure of the other half of the molecule is almost completely conserved, except the insertion of two extra strands instead of loops in LTA4 hydrolase. The structural homology between Bchl a, a protein involved in light harvesting, and LTA4 hydrolase was certainly unexpected. In LTA4 hydrolase, the function of the N-terminal domain is not yet known, but one may speculate that it participates in binding to hydrophobic molecules or surfaces with a possible regulatory function. In mammalian 15-lipoxygenase, a similar function was proposed for an N-terminal \beta-barrel domain with structural homology to a corresponding C-terminal domain in mammalian lipases (Gillmor. S.A., Villasenor, A., Fletterick, R., Sigal, E. & Browner, M.F. Nature Struc. Biol. 4, 1003-1009 (1997)).

The connection from the N-terminal to the catalytic domain is very short, a strand from the 4 stranded β-sheet connects into a strand of a 5-stranded anti-parallel β-sheet of the catalytic domain. The two sheets are closely packed and the interface is mainly hydrophobic in character with 14 hydrophobic residues contributing from the N-terminal domain and 11 from the catalytic domain. Hydrogen bonds occur between Gln116 and Ser264, Ser124 and Gln226, the backbone of Ser124 and Glu223, the backbone of Ser151 and Lys309, Lys153 and the backbone of Leu305 and indirectly through a water molecule between Tyr130 and the back-

bone of Val260. Two salt-bridges between His139 and Asp375 and between Arg174 and Asp257 complete the interactions made in this interface.

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4.3 The catalytic domain contains the zinc binding site and is structurally similar to thermolysin

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The structure of the catalytic domain (res. 210-450) is surprisingly similar to the structure of thermolysin (Fig. 5a & b) (Holmes, M. & Matthews, B. J. Mol. Biol. 160, 623-639 (1982)). When the amino acid sequence in this domain was compared with that of thermolysin, the sequence identity was found to be very low (essentially confined to the zinc binding motifs). However, the structural homology stretches out over the whole domain. Thus, no less than 146 Ca positions overlap with an r.m.s. deviation of 1.946 Å. Like thermolysin, the catalytic domain consists of two lobes, one mainly a-helical and one mixed a/b lobe. The a-lobe consists of 6 major helices interconnected by long loops containing smaller helical segments, while the a/b lobe has a 5 stranded mixed β-sheet lined with 3 helices on one side. The zinc binding site is found in between the two lobes. Since this domain contains only 245 amino acids and thermolysin contains 314 residues, some truncations have taken place, especially in the a/b lobe in which the N-terminal extended b structure is truncated and only a mixed 5 stranded β-sheet remains. The changes in the a-lobe are smaller. Here the long meandering loop 181 to 221 has been replaced by a long a-helix and the b-hairpin from 245 to 258 has been deleted.

A loop in extended conformation on the surface of the protein from 451 to 463 connects the catalytic domain with the C-terminal domain. Interestingly, this segment contains a highly conserved proline rich motif P451-G-f-P-P-x-K-P-x-Y460 which bears some resemblance to an SH3 domain recognition sequence. However, the canonical arginine residue is not present on either side of the proline motif. Nevertheless, since this stretch of amino acids is exposed on the surface of the protein, it is still possible that it could serve as an anchoring site for protein-protein interactions.

The C-terminal domain (464-610) is composed of 9 a-helices that form an unusual coil of helices reminiscent of the ones found in lytic transglycosylase⁴⁰ and

recently in the armadillo repeat region of b-catenin (Huber, A.H., Nelson, W.J. & Weis, W.I. Cell 90, 871-882 (1997)) (Fig. 6). The helices pack into two layers of parallel helices (5 inner and 4 outer helices) and in an anti-parallel manner between the two layers. The arrangements found in the two other proteins are much larger and form super-helical structures. In the C-terminal domain of LTA4 hydrolase, the arrangement is more straight and has a very compact shape. One of the helices is deformed and one of the interconnecting loops is long and contains a small 310 helix. The domain makes contacts with both the a-lobe of the catalytic domain and one of the edges of the N-terminal domain. It is positioned in a way such that the helices lie perpendicular to the 7 stranded b-sheet of the N-terminal domain and to most of the helices in the catalytic domain. The helices are amphipatic in character, with the hydrophobic sides towards the middle of the domain and hydrophilic residues pointing towards the solvent and into the deep cleft in the middle of the whole molecule. This side of the cleft is highly polar; 10 Arg and Lys residues and 4 Asp and Glu residues are positioned on this side.

4.4 Zinc coordination

The immediate surroundings of the active site Zn²⁺ ion are very similar in thermolysin and LTA4 hydrolase. The Zn²⁺ is bound between the two lobes and is coordinated by His295, His299, one carboxylic oxygen of Glu318 and the carbonyl and hydroxyl oxygens of the inhibitor bestatin so that a square based pyramid is formed. The two histidines originate from a long a-helix and the glutamate from a neighboring a-helix, all in the a-lobe. Glu296 and Tyr383, two residues implicated in the reaction mechanism for the peptide cleaving activity, are located near the Zn ion. Glu296, the putative general base, is positioned next to the metal ligand His295 and bends over the bestatin molecule and Tyr383, which was described as a proton

Interestingly, the second layer around the Zn ion shows differences between thermolysin and LTA4 hydrolase. In both enzymes the orientation of the zinc binding ligands is fixed by hydrogen bonds, however the hydrogen bond acceptors are positioned differently. In thermolysin, the Nd1 of His142 is hydrogen bonded to the

donor, also makes contact with the bestatin molecule (Figure 8a).

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Od2 of Asp170, while in LTA4 hydrolase the Nd1 of His295 is hydrogen bonded to the Oe1 of Glu325. This residue comes from a structural equivalent to the helix carrying Asp170 in thermolysin, but is shifted half a turn outwards. The Nd1 of His146 in thermolysin is hydrogen bonded to the Od1 of Asn165. This residue is part of the zinc binding signature and is conserved between the two enzymes. However, in LTA4 hydrolase the helix in which this conserved residue is placed has been rotated slightly and Asn317 is no longer making a hydrogen bond to His299. The orientation of His299 is now fixed by a hydrogen bond from the Nd1 to the carbonyl backbone oxygen of Thr302. The Od1 of Asn317 makes instead a hydrogen bond to the backbone amide of Asn381 while the Nd2 makes a hydrogen bond to the hydroxyl group of Tyr200. The last protein-ligand, Glu166 is in thermolysin hydrogen bonded to Tyr157 and a water molecule, in LTA4 hydrolase, Glu318 is only hydrogen bonded to a water molecule (Fig. 7).

4.5 Bestatin binding

Although the zinc binding site is formed by residues only from the catalytic domain and most catalytic residues also come from this domain, the active site itself is surrounded by loops from all three domains. The binding of bestatin reflects this, since it makes interactions with residues from all three domains. The main interactions of bestatin are made through the carbonyl and hydroxyl oxygens to the Zn atom. Hydrophobic interactions are made between the phenyl moiety and the phenyl rings of Tyr267, Phe316, Tyr378 and Tyr383. Also, Met270 and Gln136 are involved (Fig. 8a). The other end of the inhibitor is pointing towards the solvent, the leucine moiety makes interactions with Val292 and His295, while the carboxylic oxygens make interactions with Arg563 and Lys565 through water molecules as well as hydrogen bonds to the backbone nitrogen atoms of Gly268 and Gly269. Hydrogen bonds are formed between the peptidyl N of bestatin and Oe2 of Glu296 and between the terminal NH2 and the Oe1 of Glu271 and Oe1 of Gln136. The hydroxyl oxygen makes apart from the interaction with the Zn ion also an interaction to the OH of Tyr383. (For schematic overview see Fig. 8b). Tyr378 which gets modified during suicide inactivation sits slightly further away, but makes a hydro-

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gen bond to Tyr383 and some hydrophobic interactions with the phenyl ring of the inhibitor. These two tyrosine are both found on the same stretch of amino-acids that in thermolysin form a long a helix, however in leukotriene hydrolase this helix is interrupted and two turns of the helix are replaced by three residues (378-380) in an extended conformation. The binding of bestatin is quite different as was found in the complex between bestatin and bovine lens leucine amino-peptidase (blLAP) (Burley, S., David, P., Sweet, R., Taylor, A. & Lipscomb, W. J. Mol. Biol. 224, 113-140 (1992)). In that complex, bestatin was bound to the Zn by both the terminal nitrogen and the nonproteinaceous P1 hydroxyl oxygen, while in LTA4 hydrolase the bestatin is bound by the hydroxyl and carbonyl oxygens. The terminal nitrogen is involved in hydrogen bonding to Glu271 and Gln136. These differences could stem from the fact the blLAP is a bimetal protein with a different reaction mechanism. Moreover the binding of bestatin as seen in LTA4 hydrolase is similar with the complexes formed between thermolysin and hydroxamates which also act as bidentate ligands by the hydroxyl and carbonyl oxygens (Holmes, M. & Matthews, B. Biochemistry 20 (1981)).

35 20 40 Behind the pocket in which the phenyl ring of bestatin binds, there is a cavity that stretches 15 Å deeper into the protein and is approximately 6 to 7 Å wide. In the present structure this cavity is filled with water molecules. It has however a very hydrophobic nature and is lined with Trp311, Phe314, Trp315 Phe362, Leu365, Val367, Leu369, Pro374, Ala377, Tyr378, and Pro382. Most of these residues are strictly conserved or conserved in nature in all LTA4 hydrolase sequences known up until now, with the exception of Val367, which is replaced by a Gln in the yeast and C. elegans sequences. Interestingly space for this cavity is partly created by the interruption by the extended conformation in the stretch where Tyr378 and Tyr383 are found. One patch of this binding site is quite hydrophilic with Asn134, Asp375 and the OH of Tyr267 clustering together. This bigger cavity could be a binding site for the LTA4 substrate molecule. If the epoxide moiety would bind in a similar way as the carbonyl oxygen of bestatin to the Zn ion, then the hydrophobic tail would fit snugly into the binding site now occupied by the phenyl group of bestatin and

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would continue into the deeper hydrophobic cavity (Fig. 9a). The other tail would sit in the pocket that is now occupied by the carboxy group of bestatin and it would be long enough for the carboxylic acid to make direct electrostatic interactions with the conserved Arg563 and Lys565. 10

> The replacement of Val367 by Gln as seen in the enzyme from yeast would make the hydrophobic channel shorter and this might be one of the reasons why the yeast enzyme has a poor leukotriene A4 epoxide hydrolase activity. The manner in which the leukotriene molecule would bind is similar as what is proposed for binding of arachidonic acid in 15-lipoxygenase (Gillmor, S.A., Villasenor, A., Fletterick, R., Sigal, E. & Browner, M.F. Nature Struc. Biol. 4, 1003-1009 (1997)) with the hydrophobic end buried inside the protein and the carboxylic acid more towards the surface making interactions with Arg and Lys residues.

> The binding of bestatin acts also as a guide for the binding of peptide substrate molecules. From systematic binding studies with tri-peptides it was shown that the enzyme has a strong preference for an arginine residue as the N-terminal residue and for several tri-peptides the enzyme has a kcat/Km ratio 10-fold the kcat/Km for LTA4 (Örning, L., Gierse, J.K. & Fitzpatrick, F.A. J. Biol. Chem. 269, 11269-11273 (1994). If we roughly model a peptide in the active site with an N-terminal Arg with the carbonyl oxygen sitting on the place of the hydroxyl group of bestatin, then the Arg side-chain of this residue would sit in the same place as the phenyl group of the bestatin with the guanidinium headgroup interacting with the conserved Asp375 and the OH of Tyr267 and the more hydrophobic Cb, Cd and Cg atoms making similar interactions as the phenyl ring. The terminal aminogroup could make the same electrostatic interaction as the terminal aminogroup of bestatin with Asp271 and Gln136. This mode of binding of bestatin is in contrast with the mode proposed by Örning, since the phenyl ring seems to occupy the S1 pocket. We also propose that the LTA4 substrate molecule is occupying all three pockets, S1, S'1 and S'2.

> If the binding mode of peptides in LTA4 hydrolase is compared with the one described for thermolysin, a number of differences are observed. In thermolysin, the

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peptide molecule is held in place by many interactions to the main chain atoms provided by Asn112, Ala203, Arg203 and Trp115. None of these residues or equivalent residues can be found in the binding site in LTA4 hydrolase. Furthermore, although binding pockets S1 and S'1 are at similar positions as in thermolysin, site S'2 has to be different since its space is occupied by Tyr378 in LTA4 hydrolase. Glu271 and Gln136 and the N-terminal domain are filling up the space into which in thermolysin the upstream peptide binds contributing to the exo-peptidase function instead of an endo-peptidase function as in thermolysin.

4.6 Putative Phosphorylation site

Recently specific phosphorylation by a yet unknown specific kinase of Ser415 has been described as means of regulation of LTA4 hydrolase activity in endothelial cells (Rybina, I.V., Liu, H., Gor, Y. & Feinmark, S.J. *J Biol Chem* 272, 31865-71 (1997)). This residue is conserved in all mammalian LTA4 hydrolases and is embedded in a highly homologous stretch of residues. Phosphorylation of this residue seems to inhibit the epoxide hydrolase activity but not the amino-peptidase activity. In the structure this residue is located in a loop connecting two a-helices that lie on the surface of the molecule. The loop itself is located at the back of the enzyme.

4.7 Aminopeptidase activity

The amino-peptidase activity catalyzed by this enzyme has been well studied and many of the important residues have been target for site-directed mutagenesis work. This lead to a proposal in which Glu296 would act as a general base (Wetterholm, A., et al. Proc Natl Acad Sci U S A 89, 9141-9145 (1992)) and Tyr383 as a putative proton donor (Blomster, M., Wetterholm, A., Mueller, M.J. & Haeggström, J.Z. Eur. J. Biochem. 231, 528-534 (1995)). In the current complex, these residues are involved in hydrogen bonds with the bestatin molecule. If bestatin binding is seen as a rough analog for the transition state binding, then the interaction of Glu296 with the hydroxyl oxygen of bestatin indicates that this residue could indeed activate a water-molecule for the nucleophilic attack. The role of Tyr383 cannot so easily be confirmed, however its position strongly suggest the role of proton donor. In thermolysin the proton donor is His231 and although the Ca position of this resi-

due is 4.1Å removed from the Ca position of Tyr383 in LTA4 hydrolase, the Nd1 is only 1 Å removed from the OH position of Tyr383. The conserved Glu271 could be involved in the exo-protease activity of the protein. Recently, the analogous Glu350 in aminopeptidase N and Glu352 in aminopeptidase A were subject to site-directed mutagenesis work (Luciani, N., et al. Biochemistry 37, 686-692 (1998); and Vazeux, G., Iturrioz, X., Corvol, P. & Llorenz-Cortez, C. Biochem. J. 334, 407-413 (1998)) and it was observed that mutations of this residue lead to large decreases in the activity in the case of substitutions by conserved amino-acids such as aspartate and glutamine and absence of activity in substitution by alanine. It was concluded that Glu350 belonged to the anionic binding site in that protein. A mechanism based on thermolysin was proposed for aminopeptidase N with a pentavalent transition state with an additional interaction between the free a-aminogroup and Glu350. In this structure we can observe such an interaction between Glu271 and the free aminogroup of bestatin. Furthermore the penta-valent coordination of Zn by the His295, His299, Glu318 and the carbonyl and hydroxyl groups of bestatin indicates that this is an equivalent transition state analog complex as determined previously for thermolysin.

From careful sequence alignments and structural insight we can conclude that the enzymes in the M1 family of proteases will share a highly conserved catalytic domain that includes part of the N-terminal domain as we see it in LTA4 hydrolase and the thermolysin-like domain. There is no homology for residues in the C-terminal domain and we believe that this domain is unique for LTA4 hydrolases. According to the present invention, it is suggested that all proteases belonging to class M1 with the signature HExxH and a Glu 18 residues downstream will function in a similar way to thermolysin.

4.8 Epoxide hydrolase activity

Concerning the epoxide hydrolase activity, much less is known about the functional elements and mechanisms of catalysis. In fact, the prosthetic zinc is the only critical component identified thus far and may potentially assist in the introduction of a water molecule at C12 or in the activation of the epoxide. Although Tyr378 and

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Tvr383 are important active side residues, none of them is essential for catalysis. A mutation of Tyr378 to Phe protects the enzyme against suicide inhibition, however the specificity of the double bond configuration is partly lost (Mueller, M., Andberg, M., Samuelsson, B. & Haeggstrom, J. J. Biol. Chem. 271, 24345-24348 (1996)) since a novel metabolite with a cis-trans-cis conjugated system can be detected. Thus, Tyr378 is a major binding site for LTA4 during suicide inactivation and seems to play a role for the formation of the correct double bond geometry in the product LTB4. Mutations of Tyr383 abolish the amino-peptidase activity where it has a role as potential proton donor (vide supra) but the epoxide hydrolase activity is only decreased compared to wild-type. It is however implicated in the stereospecific introduction of water during the hydrolysis of LTA4 to LTB4 since these mutants convert LTA4 in both LTB4 and 5 [S],6 [S]-DHETE (Andberg, M., Hamberg, M. & Haeggstrom, J. J. Biol. Chem. 272, 23057-23063 (1997)). Moreover careful analysis of the catalytic properties of enzymes mutated in pos. 383, viz [Y383F], [Y383H] and [Y383Q]LTA4 hydrolase have indicated that the epoxide hydrolase reaction follows an SN1 mechanism.

If one considers the chemistry carried out by LTA4 hydrolase, the enzyme has two major tasks during the hydrolysis of LTA4 to LTB4. First introduction of a water molecule stereospecific at C12 and second to generate a cis-double bond Æ6 in the resulting conjugated triene system [cf. Fig. 1]. If LTA4 is modeled into the putative substrate binding pocket as indicated in figure 9b, the catalytic zinc gets close to the epoxide and not C12 of the substrate. Therefore the most likely role of the Zn ion is to act directly as a Lewis acid to activate and open the epoxide ring. This would generate a carbocation, whose charge will be delocalised over the conjugated triene system from C7 to C12. Since this intermediate has an sp2 hydridized planar configuration at C12, it is in principle open for nucleophilic attack from either side of the molecule. The conserved Asp375 is positioned in such a way that a water molecule bound to it is in "attacking" distance of C12 of a modeled LTA4 molecule, the position into which a hydroxyl group is inserted during the reaction.

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This will account for the proper stereo-chemical and positional insertion of the hydroxyl-group at C12 in R configuration.

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The shape and curvature of the LTA4 binding pocket also gives a clue as to how the enzyme creates the cis double bond at Æ6. Since there is free rotation between the c6 and c7 of LTA4, this bond may be kept in a "pro-cis" configuration in the transition state, which in turn would facilitate the formation of a Æ6-cis double bond form the carbocation intermediate. If LTA4 is modeled in this way, the entire molecule adopts a bent shape, fitting very well with the architecture of the binding pocket (Fig. 9b). Hence, the critical double bond geometry at Æ6 of LTB4 is probably guaranteed by the exact binding conformation of LTA4 at the active side which in turn is governed by all the structural elements participating in substrate binding, including the carboxylate recognition sites, Arg56 and Lys565, the catalytic zinc and the hydrophobic residues lining the pocket. The putative binding cleft for the leukotriene molecule is narrow and bend and thereby favoring LTA4 over other epoxides. The two tyrosines are positioned such that they are in contact with the triple double bond configuration of a modeled LTA4 molecule at the bent of the putative binding pocket and they are hydrogen-bonded to each other. Therefore their position is ideal for guidance in stereo-specificity of the double bond configuration. The loss of specificity for the hydroxyl-incorporation at the C12 position in case of the Tyr383 position can be explained that mutations at this position would possibly create extra space for a water molecule that could attack at the C6 position and thereby form 5 [S],6 [S]-DHETE.

The position of Tyr378 is such that it is in contact with the C6 atom of the modeled LTA4 molecule. If after opening of the epoxide ring the hydroxyl group of Tyr378 instead of a water molecule would attack the carbon-cation at the C6 position, a covalently attached molecule is formed which forms the suicide inhibited complex. In order to check this hypothesis and to obtain more information about the binding-site for leukotriene A4, the structure of this inhibited species would be essential.

In order to exclude the possibility that residues near the active site might have further catalytic roles in the epoxide hydrolase reaction, a thorough investigation of these residues, such as Glu271 and Gln136 has to be started. Furthermore the proposed role of Asp375 in activating a water molecule for the stereospecific attack at C12 has to be investigated.

Accordingly, the present invention has solved the first specific leukotriene converting enzyme, which for the first time reveals the binding mode for leukotriene molecules. Furthermore, insight is provided in a unique active site that harbours two activities using different amino-acids to catalyze different reactions.

5. CONFORMATIONAL DATA

Table 9: Structure coordinates	s of LTA ₄ hydrolase-thiolamine complex	

25	15	CRYST SCALE1 SCALE2 SCALE3	68.	560 0.01 0.00		(0 83. 0.00000 0.00757 0.00000	0. 0.	90.00 00000 00000)	90.00 0.00000 0.00000 0.00000	P21212
				Atom	res	. Cl	hain No	. >	٢	у	z	occ B-factor
	20	ATOM	1	N	PRO	А	1	-0.	593	16.387	63.494	1.00 97.99
		ATOM	2	CA	PRO		ī		890	16.918	63.874	1.00 97.22
		ATOM	3	C	PRO		ī		210	18.371	63.525	1.00100.00
30		ATOM	4	ō	PRO		ī		402	18.667	62.342	1.00100.00
••		ATOM	5	СВ	PRO		ī		130	16.551	65.332	1.00 97.81
	25	ATOM	6	CG	PRO		ī		221	15.355	65.583	1.00100.00
		ATOM	7	CD	PRO		ī		290	15.233	64.369	1.00 97.05
		ATOM	8	N	GLU		2		216	19.272	64.556	1.00 96.95
		ATOM	9	CA	GLU	Α	2		569	20678	64.314	1.00 95.71
		ATOM	10	С	GLU	Α	2		188	21.701	65.386	1.00 94,33
35	30	MOTA	11	0	GLU	Α	2	-2.	512	21.542	66.562	1.00 93.21
		ATOM	12	CB	GLU	Α	2	-4.	105	20.768	64.214	1.00 97.26
		ATOM	13	CG	GLU	Α	2	-4.	587	21.732	63.125	1.00100.00
		ATOM	14	CD	GLU		2	-4.	351	21.139	61.767	1.00100.00
		ATOM	15	OE1	GLU	Α	2	-3.	301	21.261	61.152	1.00100.00
	35	ATOM	16	OE2	GLU	Α	2	-5.	361	20.398	61.368	1.00100.00
40		ATOM	17	N	ILE	Α	3	-1.	550	22.799	64.944	1.00 86.29
40		ATOM	18	CA	ILE	Α	3	-1.	148	23.905	65.820	1.00 81.53
		ATOM	19	C	ILE		3	-2.	006	25.154	65.661	1.00 75.68
	40	ATOM	20	0	ILE		3		835	25.288	64.763	1.00 76.97
	40	ATOM	21	CB	ILE		3	0.	308	24.324	65.707	1.00 83.45
		ATOM	22		ILE		3		452	25.521	64.759	1.00 83.63
		MOTA	23		ILE		3		198	23.160	65.300	1.00 84.76
45		ATOM	24		ILE		3		184	25.361	63.375	1.00 91.36
	4.5	ATOM	25	N	VAL		4		725	26.099	66.523	1.00 61.54
	45	ATOM	26	CA	VAL		4		477	27.303	66.482	1.00 56.32
		ATOM	27	С	VAL		4		658	28.552	66.623	1.00 50.98
,		ATOM	28	0	VAL		4		803	28.694	67.512	1.00 47.84
		ATOM	29		VAL		4		514	27.318	67.595	1.00 58.99
	50	ATOM	30		VAL		4		735	28.754	68.047	1.00 58.40
50	50	ATOM.	31		VAL		4		819	26.691	67.131	1.00 58.56
		ATOM	32	N	ASP		5		012	29.486	65.732	1.00 39.38
		ATOM	33	CA	ASP	Α	5	-1.	403	30.782	65.763	1.00 32.64

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5		ATOM	34	Ç	ASP A	5	-2.308	31.596	66.634	1.00 36.35
		ATOM	35	0	ASP A	5	-3.343	32.051	66.171	1.00 38.30
		ATOM	36	CB	ASP A	5	-1.252	31.492	64.400	1.00 30.79
		ATOM	37	ÇG	ASP A	5	-0.251	32.581	64.563	1.00 29.96
	5	ATOM	.38	OD1	ASP A	5	-0.069	33.123	65.635	1.00 35.01
		ATOM	39	OD2	ASP A	5	0.457	32.831	63.493	1.00 29.81
10		ATOM	40	N	THR A	6	-1.931	31.745	67.903	1.00 32.32
10		ATOM	41	CA	THR A	6	-2.710	32.507	68.842	1.00 32.08
		ATOM	42	C	THR A	6	-2.701	34.011	68.557	1.00 40.63
	10	ATOM	43	0	THR A	6	-3.484	34.759	69.132	1.00 46.68
		ATOM	44	CB	THR A	6	-2.357	32.171	70.295	1.00 44.71
		ATOM	45	OG1	THR A	6	-0.967	32.322	70.505	1.00 51.05
		ATOM	46	CG2	THR A	6	-2.789	30.741	70.604	1.00 35.79
15		ATOM	47	N	CYS A	7	-1.842	34.480	67.656	1.00 32.51
,,	15	ATOM	48	CA	CYS A	7	-1.797	35.923	67.335	1.00 28.92
		ATOM	49	C	CYS A	7	-2.627	36.329	66.129	1.00 31.49
		ATOM	50	0	CYS A	7	-2.780	37.523	65.875	1.00 25.42
		ATOM	51	СВ	CYS A	7	-0.362	36.410	67.107	1.00 27.38
		ATOM	52	ŞĢ	CYS A	7	0.686	35.944	68.518	1.00 32.02
	20	ATOM	53	N	SER A	8	-3.140	35.315	65.383	1.00 34.03
20		ATOM	54	CA	SER A	8	-3.940	35.508	64.158	1.00 32.97
		ATOM	55	С	SER A	В	-5.410	35.136	64.264	1.00 33.52
		ATOM	56	0	SER A	8	-5.744	34.137	64.866	1.00 32.89
		ATOM	57	CB	SER A	8	-3.363	34.754	62.980	1.00 34.07
	25	ATOM	58	OG	SER A	8	-4.017	35.182	61.798	1.00 36.65
		ATOM	59	N	LEU A	9	-6.289	35.921	63.635	1.00 30.79
		ATOM	60	CA	LEU A	9	-7.724	35.649	63.672	1.00 31.91
25		ATOM	61	C	LEU A	9	-8.198	35.009	62.377	1.00 36.07
		ATOM	62	0	LEU A	9	-9.359	34.626	62.216	1.00 38.61
	30	ATOM	63	СВ	LEU A	9	-8.514	36.958	63.874	1.00 32.47
		ATOM	64	CG	LEU A	9	-8.306	37.688	65.212	1.00 35.39
		ATOM	65	CD1	LEU A	9	-9.113	38.983	65.193	1.00 32.27
		ATOM	66	CD2	LEU A	9	-8.746	36.816	66.397	1.00 33.25
		MOTA	67	N	ALA A	10	-7.273	34.933	61.443	1.00 28.63
30	35	MOTA	68	CA	ALA A	10	-7.545	34.408	60.147	1.00 27.14
		MOTA	69	С	ALA A	10	-7.643	32.921	60.090	1.00 34.34
		ATOM	70	0	ALA A	10	-7.296	32.173	61.005	1.00 37.34
		MOTA	71	CB	ALA A	10	-6.551	34.936	59.100	1.00 27.72
		MOTA	72	N	SER A	11	-8.130	32.503	58.959	1.00 32.08
	40	MOTA	73	CA	SER A	11	-8.256	31.115	58.708	1.00 32.03
35		MOTA	74	С	SER A	11	-6.838	30.519	58.656	1.00 32.67
55		ATOM	75	0	SER A	11	-5.927	31.028	57.986	1.00 29.29
		MOTA	76	CB	SER A	11	-9.013	30.934	57.401	1.00 38.42
		MOTA	77	OG	SER A	11	-10.391	30.728	57.648	1.00 44.17
	45	MOTA	78	N	PRO A	12	-6.651	29.440	59.387	1.00 29.14
		ATOM	79	CA	PRO A	12	-5.370	28.786	59.476	1.00 26.83
		MOTA	80	С	PRO A	12	-4.935	28.176	58.173	1.00 32.64
40		ATOM	81	0	PRO A	12	-5.737	28.007	57.284	1.00 35.89
		ATOM	82	CB	PRO A	12	~5.544	27.698	60.540	1.00 28.28
	50	ATOM	83	CG	PRO A	12	-7.029	27.571	60.843	1.00 32.92
		ATOM	84	CD	PRO A	12	-7.731	28.587	59.952	1.00 30.42
		ATOM	85	N	ALA A	13	-3.645	27.836	58.063	1.00 30.63
		MOTA	86	CA	ALA A	13	-3.066	27.236	56.855	1.00 28.36
		ATOM	87	С	ALA A	13	-3.644	25.852	56.576	1.00 33.99
45	55	MOTA	88	0	ALA A	13	-3.455	25.240	55.528	1.00 31.60
		MOTA	89	CB	ALA A	13	-1.561	27.133	57.050	1.00 27.68
		MOTA	90	N	SER A	14	-4.338	25.352	57.571	1.00 31.10
		ATOM	91	CA	SER A	14	-4.919	24.069	57.469	1.00 30.66
		MOTA	92	С	SER A	14	-6.242	24.133	56.753	1.00 37.86
	60	ATOM	93	0	SER A	14	-6.768	23.118	56.328	1.00 45.79
50		ATOM	94	CB	SER A	14	-5.005	23.386	58.825	1.00 34.33
50		ATOM	95	OG	SER A	14	-6.006	23.978	59.621	1.00 41.01
		ATOM	96	N	VAL A	15	-6.785	25.327	56.630	1.00 32.80
		ATOM	97	CA	VAL A	15	-8.036	25.529	55.917	1.00 31.81

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5		ATOM ATOM	98 99	С 0	VAL		15	-7.777	26.107	54.507		34.70
		ATOM	100	СВ	VAL		15 15	-8.241 -9.033	25.576 26.336	53.494 56.720		31.96
		ATOM	101		VAL		15	-10.272	26.638	55.861		33.31
	5	ATOM	102		VAL		15	-9.412	25.538	57.949		30.32
		ATOM	103	N	CYS	Α	16	-6.990	27.183	54.453		33.85
40		ATOM	104	CA	CYS	Α	16	-6.602	27.826	53.189		38.27
10		ATOM	105	С	CYS		16	-5.206	28.388	53.265	1.00	37.14
	10	ATOM	106	0	CYS		16	-4.616	28.534	54.322		39.70
	10	ATOM	107	CB	CYS		16	-7.589	28.870	52.581		42.09
		ATOM ATOM	108 109	SG N	CYS ARG		16 17	-7.844 -4 .679	30.418 28.722	53.540 52.132		47.38
		ATOM	110	CA	ARG		17	-3.349	29.262	52.132		32.10 32.54
		ATOM	111	C	ARG		17	-3.210	30.307	51.005		34.56
15	15	ATOM	112	0	ARG		17	-3.511	30.065	49.842		35.07
		ATOM	113	CB	ARG	Α	17	-2.371	28.152	51.758		36.83
		ATOM	114	ÇĞ	ARG		17	-1.779	27.391	52.915	1.00	40.61
		ATOM	115	CD	ARG		17	-1.472	25.970	52.503		27.18
	20	ATOM	116	NE	ARG		17	-1.963	25.026	53.501		52.41
	20	ATOM ATOM	117 118	CZ	ARG ARG		17 17	-1.244	24.036	54.035		69.41
20		ATOM	119		ARG		17	0.020 -1.810	23.812 23.246	53.683 54.952		54.86
		ATOM	120	N	THR		18	-2.711	31.454	51.378		49.68
		ATOM	121	CA	THR		18	-2.489	32.477	50.428		26.12
	25	ATOM	122	С	THR		18	-1.250	32.110	49.653		30.83
		ATOM	123	0	THR	Α	18	-0.174	31.964	50.194		29.06
		ATOM	124	CB	THR		18	-2.276	33.810	51.134		34.27
25		MOTA	125		THR		18	-3.481	34.261	51.738		32.95
	30	ATOM	126		THR		18	-1.730	34.839	50.156		35.91
	30	ATOM ATOM	127 128	N CA	LYS		19	-1.408	31.955	48.365		31.55
		ATOM	129	CA	LYS LYS		19 19	-0.298 0.359	31.615 32.848	47.511 46.906		31.74 33.90
		ATOM	130	ō	LYS		19	1.513	32.834	46.520		34.57
		ATOM	131	СВ	LYS		19	-0.795	30.697	46.398		36.08
30	35	ATOM	132	CG	LYS		19	-1.332	29.368	46.924		62.54
		ATOM	133	CD	LYS	Α	19	-0.281	28.257	47.057		82.23
		ATOM	134	CE	LYS		19	0.093	27.880	48.496	1.00	77.50
		ATOM	135	ΝZ	LYS		19	1.553	27.849	48.745		55.63
	40	MOTA	136	N	HIS		20	-0.387	33.928	46.810		31.40
	40	ATOM ATOM	137 138	CA C	HIS HIS		20 20	0.160 -0.655	35.122	46.198		29.22
35		ATOM	139	Ö	HIS		20	-1.833	36.345 36.239	46.517 46.846		34.68 35.34
		ATOM	140	СВ	HIS		20	0.123	34.956	44.666		26.47
		MOTA	141	CG	HIS		20	0.865	36.022	43.970		26.77
	45	MOTA	142	ND1	HIS	Α	20	2.249	36.046	43.980		28.92
		MOTA	143	CD2	HIS	Α	20	0.415	37.091	43.280	1.00	27.43
		ATOM	144		HIS		20	2.622	37.126	43.301	1.00	28.21
40		ATOM	145		HIS		20	1.536	37.781	42.865		28.18
	50	ATOM ATOM	146 147	N CA	LEU		21	0.000	37.492	46.390		30.14
	50	ATOM	148	CA	LEU LEU		21 21	-0.596 -0.134	38.782	46.610		31.02
		ATOM	149	õ	LEU		21	1.073	39.786 39.952	45.562 45.312		38.34 37.30
		ATOM	150	СВ	LEU		21	-0.342	39.363	47.999		31.30
		ATOM	151	CG	LEU		21	-0.611	40.880	48.047		32.33
45	55	ATOM	152		LEU		21	-2.088	41.192	48.324		27.10
		MOTA	153		LEU		21	0.277	41.522	49.100		32.86
		ATOM	154	N	HIS		22	-1.127	40.442	44.951		35.47
		ATOM	155	CA	HIS		22	-0.895	41.452	43.920		34.24
	60	ATOM ATOM	156 157	C	HIS		22	-1.249	42.742	44.550		33.99
	00	ATOM	158	O CB	HIS HIS		22 22	-2.402 -1.720	42.957	44.905		35.72
50		ATOM	159	CG	HIS		22	-1.350	41.244 42.256	42.624 41.615		33.38
		ATOM	160		HIS		22	-0.030	42.576	41.384		38.81
		ATOM	161		HIS		22	-2.125	43.043	40.830		39.07

5		MOTA	162	CE1	HIS A	22	-0.019	43.534	40.462	1.00 38.66
		ATOM	163	NE2	HIS A	22	-1.262	43.829	40.103	1.00 39.13
		MOTA	164	N	LEU A	23	-0.235	43.539	44.757	1.00 30.17
		ATOM	165	CA	LEU A	23	-0.416	44.793	45.405	1.00 33.32
	5	ATOM	166	С	LEU A	23	-0.203	45.949	44.440	1.00 44.46
		ATOM	167	0	LEU A	23	0.828	46.068	43.761	1.00 44.06
		ATOM	168	CB	LEU A	23	0.446	44.882	46.680	1.00 33.72
10		MOTA	169	CG	LEU A	23	-0.141	45.682	47.871	1.00 33.15
		ATOM	170		LEU A	23	0.780	46.835	48.172	1.00 26.07
	10	ATOM	171		LEU A	23	-1.539	46.213	47.609	1.00 35.39
		MOTA	172	N	ARG A	24	-1.256	46.765	44.395	1.00 42.83
		ATOM	173	CA	ARG A	24	-1.406	47.964	43.596	1.00 42.03
		ATOM	174	c	ARG A	24	-1.930	49.005	44.562	1.00 39.15
		ATOM	175	Ö	ARG A	24	-3.025	48.859	45.107	1.00 39.13
15	15	ATOM	176	СВ	ARG A	24	-2.458	47.716	42.504	
	13	ATOM	177	CG		24				1.00 46.35
					ARG A		-2.054	46.750	41.382	1.00 50.50
		ATOM	178	CD	ARG A	24	-2.754	47.058	40.043	1.00 80.27
		ATOM	179	NE	ARG A	24	-4.200	46.798	40.062	1.00 95.12
	20	MOTA	180	CZ	ARG A	24	-5.152	47.703	39.826	1.00100.00
	20	ATOM	181		ARG A	24	-4.863	48.973	39.483	1.00100.00
20		ATOM	182		ARG A	24	-6.432	47.326	39.865	1.00100.00
		ATOM	183	N	CYS A	25	-1.164	50.028	44.844	1.00 32.39
		MOTA	184	CA	CYS A	25	-1.698	50.969	45.813	1.00 33.30
		ATOM	185	С	CYS A	25	-1.061	52.325	45.724	1.00 34.82
	25	ATOM	186	0	CYS A	25	-0.012	52.514	45.076	1.00 31.03
		ATOM	187	СВ	CYS A	25	-1.503	50.440	47.257	1.00 34.67
		ATOM	188	SG	CYS A	25	0.231	50.529	47.798	1.00 38.07
25		ATOM	189	N	SER A	26	-1.711	53.257	46.418	1.00 34.39
20		ATOM	190	CA	SER A	26	-1.196	54.601	46.437	1.00 34.33
	30	ATOM	191	C	SER A	26	-0.963	55.133	47.821	1.00 30.77
	-	ATOM	192	ŏ	SER A	26	~1.738	54.853	48.757	1.00 37.56
		ATOM	193	CB	SER A	26	-1.889			
		ATOM	194	OG	SER A	26	-0.899	55.600 56.330	45.530	1.00 42.70
		ATOM	195						44.824	1.00 61.74
30	35			N	VAL A	27	0.133	55.897	47.886	1.00 39.43
30	33	ATOM	196	CA	VAL A	27	0.624	56.583	49.081	1.00 41.31
		ATOM	197	С	VAL A	27	0.209	58.043	49.082	1.00 44.32
		ATOM	198	0	VAL A	27	0.562	58.799	48.187	1.00 45.24
		ATOM	199	CB	VAL A	27	2.135	56.531	49.207	1.00 46.35
	40	ATOM	200		VAL A	27	2.524	57.207	50.522	1.00 45.62
	40	ATOM	201		VAL A	27	2.592	55.079	49.178	1.00 47.20
25		ATOM	202	N	ASP A	28	-0.553	58.417	50.093	1.00 37.94
35		ATOM	203	CA	ASP A	28	-1.040	59.764	50.237	1.00 35.28
		ATOM	204	С	ASP A	28	-0.595	60.366	51.538	1.00 33.85
		ATOM	205	0	ASP A	28	-1.181	60.099	52.598	1.00 28.52
	45	ATOM	206	CB	ASP A	28	-2.559	59.807	50.189	1.00 37.09
		MOTA	207	CG	ASP A	28	-3.055	61.205	50.095	1.00 55.20
		ATOM	208	OD1	ASP A	28	-2.611	62.119	50.767	1.00 59.17
40		ATOM	209		ASP A	28	-3.993	61.335	49.192	1.00 61.41
40		ATOM	210	N	PHE A	29	0.436	61.174	51.405	1.00 36.42
	50	ATOM	211	CA	PHE A	29	1.044	61.888	52.512	1.00 43.07
		ATOM	212	C	PHE A	29	0.105	62.928	53.077	
		ATOM	213	ŏ	PHE A	29	0.161	63.279	54.257	1.00 51.14
		ATOM	214	СВ	PHE A	29	2.410			1.00 51.35
		ATOM	215	CG	PHE A			62.517	52.143	1.00 47.77
	55	ATOM	216			29	3.519	61.485	52.079	1.00 50.86
45	<i></i>				PHE A	29	4.066	60.957	53.247	1.00 52.08
		ATOM	217		PHE A	29	3.996	61.001	50.863	1.00 53.94
		ATOM	218		PHE A	29	5.075	59.995	53.215	1.00 52.83
		ATOM	219		PHE A	29	5.013	60.046	50.813	1.00 56.46
	~ 0	ATOM	220	CZ	PHE A	29	5.559	59.538	51.992	1.00 53.39
	60	ATOM	221	N	THR A	30	-0.766	63.420	52.220	1.00 47.10
		ATOM	222	CA	THR A	30	-1.718	64.386	52.654	1.00 45.48
50		ATOM	223	С	THR A	30	-2.788	63.715	53.509	1.00 48.41
		MOTA	224	0	THR A	30	-3.045	64.082	54.649	1.00 48.64
•		ATOM	225	CB	THR A	30	-2.283	65.097	51.434	1.00 54.06
				-						

5		MOTA	226	OG1	THR	А	30	-1.428	66.186	51.107	1.00 50.68
		ATOM	227		THR		30	-3.697	65.568	51.745	1.00 60.28
		ATOM	228	N	ARG		31	-3.392	62.683	52.978	1.00 46.66
		ATOM	229	CA	ARG	А	31	-4.404	61.987	53.734	1.00 47.88
	5	ATOM	230	С	ARG	A	31	-3.826	60.999	54.750	1.00 45.46
		ATOM	231	0	ARG	A	31	-4.590	60.468	55.551	1.00 41.52
		ATOM	232	CB	ARG	А	31	-5.335	61.214	52.805	1.00 56.73
10		MOTA	233	CG	ARG	A	31	-5.950	62.065	51.700	1.00 84.16
		ATOM	234	CD	ARG	А	31	-7.338	61.568	51.284	1.00100.00
	10	ATOM	235	NE	ARG	A	31	-7.344	60.450	50.327	1.00100.00
		ATOM	236	CZ	ARG		31	-8.148	60.371	49.251	1.00100.00
		ATOM	237		ARG		31	-9.034	61.324	48.944	1.00100.00
		ATOM	238		ARG		31	-8.062	59.298	48.460	1.00100.00
15	15	ATOM	239	N	ARG		32	-2.489	60.752	54,683	1.00 39.71
••	13	ATOM	240	CA	ARG		32	-1.751	59.798	55.531	1.00 39.09
		ATOM	241	C	ARG		32	-2.324	58.411	55.379	1.00 39.62
		ATOM	242	O	ARG		32	-2.495	57.655	56.337	1.00 33.10
		ATOM	243 244	CB	ARG		32	-1.523	60.115	57.022	1.00 37.14
	20	ATOM ATOM	244	CG	ARG ARG		32 32	-1.197 0.277	61.569	57.337	1.00 71.25
	20	ATOM	245	NE	ARG		32	0.703	61.834	57.686	1.00100.00
20		ATOM	247	CZ	ARG		32	1.284	61.299 62.005	58.986 59.961	1.00100.00 1.00 79.51
		ATOM	248		ARG		32	1.522	63.308	59.831	1.00 79.31
		ATOM	249		ARG		32	1.626	61.387	61.098	1.00 44.96
	25	ATOM	250	N	THR		33	-2.612	58.068	54.139	1.00 39.83
		ATOM	251	CA	THR		33	-3.162	56.752	53.902	1.00 39.31
		ATOM	252	C	THR		33	-2.543	56.010	52.760	1.00 41.13
25		ATOM	253	ō	THR		33	-1.853	56.574	51.926	1.00 42.93
25		ATOM	254	СВ	THR		33	-4.635	56.835	53.641	1.00 43.44
	30	ATOM	255		THR		33	-4.798	57.636	52.468	1.00 40.17
		ATOM	256		THR		33	-5.245	57.468	54.880	1.00 38.71
		ATOM	257	N	LEU	Α	34	-2.822	54.717	52.762	1.00 35.26
		ATOM	258	CA	LEU	Α	34	-2.372	53.799	51.745	1.00 35.20
		ATOM	259	С	LEU	A	34	-3.632	53.293	51.098	1.00 32.49
30	35	ATOM	260	0	LEU	A	34	-4.474	52.670	51.751	1.00 30.96
		ATOM	261	CB	LEU		34	-1.522	52.651	52.322	1.00 37.07
		MOTA	262	CG	LEU		34	-0.149	52.571	51.685	1.00 42.99
		MOTA	263		LEU		34	0.648	51.425	52.285	1.00 40.58
	40	ATOM	264		LEU		34	-0.360	52.302	50.208	1.00 50.83
	40	ATOM	265	N	THR		35	-3.800	53.632	49.838	1.00 28.72
35		ATOM	266	CA	THR		35	-5.017	53.228	49.198	1.00 31.26
00		ATOM	267	C	THR		35	-4.838	52.329	48.013	1.00 36.54
		MOTA MOTA	268 269	O CB	THR		35	~3.940 -5.877	52.546	47.187	1.00 34.70
	45	ATOM	270	OG1	THR		35 35	-5.877 -5.484	54.427 55.549	48.813 49.579	1.00 44.88
	70	ATOM	271		THR		35	-7.324	54.094	49.109	1.00 58.59 1.00 49.42
		ATOM	272	N	GLY		36	-5.726	51.329	47.950	1.00 32,57
0.2		ATOM	273	CA	GLY		36	-5.696	50.405	46.837	1.00 33.89
40		ATOM	274	c	GLY		36	-6.418	49.074	46.993	1.00 34.50
	50	ATOM	275	0	GLY		36	-7.441	48.919	47.678	1.00 31.78
		ATOM	276	N	THR		37	-5.836		46.293	1.00 35.93
		MOTA	277	CA	THR		37	-6.327	46.723	46.281	1.00 36.12
		ATOM	278	С	THR		37	-5.268	45.696	46.473	1.00 35.67
		MOTA	279	0	THR	А	37	-4.155	45.795	45.964	1.00 33.86
45	55	MOTA	280	CB	THR	Α	37	-7.119	46.306	45.050	1.00 42.21
		ATOM	281	OG1	THR	Α	37	-6.507	46.804	43.870	1.00 30.98
		ATOM	282	CG2	THR	Α	37	-8.547	46.793	45.229	1.00 50.03
		ATOM	283	N	ALA	A	38	-5.687	44.705	47.220	1.00 32.95
		ATOM	284	CA	ALA		38	-4.886	43.570	47.533	1.00 33.45
	60	MOTA	285	С	ALA		38	-5.481	42.374	46.824	1.00 35.47
		ATOM	286	0	ALA		38	-6.580	41.906	47.151	1.00 32.91
50		MOTA	287	CB	ALA		38	-4.845	43.341	49.044	1.00 33.72
		MOTA	288	N	ALA		39	-4.764	41.874	45.834	1.00 32.70
		ATOM	289	CA	ALA	Α	39	-5.274	40.702	45.140	1.00 31.59

5		ATOM	290	С	ALA A	ь а	9	-4.692	39.464	45.770	1 00	32.11
		ATOM	291	ŏ	ALA 2		9	-3.514	39.147	45.608		32.46
		ATOM	292	СВ	ALA A		9	-4.934	40.729	43.662		32.13
		ATOM	293	N	LEU A		0	-5.505	38.774	46.508		27.06
	5	ATOM	294	CA	LEU A	A 4	0	-5.001	37.593	47.155		29.04
		ATOM	295	С	LEU A	A 4	0	-5.331	36.322	46.364		36.88
		ATOM	296	0	LEU A	A. 4	0	-6.485	36.100	45.963		28.89
10		ATOM	297	CB	LEU A	A 4	0	-5.587	37.451	48.600	1.00	29.39
		ATOM	298	CG	LEU A	A. 4	0	-5.303	38.598	49.559	1.00	31.39
	10	ATOM	299	CD1	LEU A	A 4	0	-5.435	38.063	50.970	1.00	32.62
		ATOM	300	CD2	LEU /	A 4	0	-3.879	39.019	49.355	1.00	31.60
		MOTA	301	N	THR A	A 4	1	-4.310	35.470	46.165	1.00	42.40
		ATOM	302	CA	THR A		1	-4.523	34.210	45.488	1.00	43.93
15		ATOM	303	С	THR A		1	-4.548	33.155	46.552	1.00	43.75
10	15	ATOM	304	0	THR A		1	-3.510	32.827	47.115	1.00	45.22
		MOTA	305	CB	THR A	A 4	1	-3.511	33.892	44.402		55.44
		MOTA	306		THR A		1	-3.604	34.885	43.418		55.57
		MOTA	307		THR A		1	-3.872	32.544	43.802		47.78
	00	ATOM	308	N	VAL 2		2	-5.755	32.688	46.848		33.25
	20	ATOM	309	CA	VAL A		2	-5.946	31.720	47.893		32.21
20		ATOM	310	С	VAL		2	-6.166	30.312	47.380		40.56
		ATOM	311	0	VAL		2	-6.827	30.105	46.376		42.56
		ATOM	312	CB	VAL		2	-7.017	32.153	48.920		36.45
	25	ATOM	313		VAL		2	-6.817	31.451	50.266		36.89
	25	ATOM	314		VAL		2	-6.963	33.665	49.170		36.10
		ATOM	315	N	GLN A		13	-5.590	29.357	48.117		35.91
		ATOM	316	CA	GLN A		3	-5.678	27.945	47.838		31.59
25		ATOM	317	C	GLN A		13	-6.346	27.244	48.988		38.98
	30	MOTA	318	0	GLN I		13	-5.916	27.317	50.144		40.92
	30	ATOM	319	CB	GLN A		13	-4.305	27.319	47.568		30.50
		ATOM	320	CG	GLN A		13	-4.362	25.800	47.259		53.80
		MOTA	321	CD	GLN A		3	-2.986	25.177	47.099		62.47
		ATOM ATOM	322 323		GLN A		13	-2.569 -2.274	24.842	45.978		57.34
30	35	ATOM	324	NEZ				-7.423	25.037 26.555	48.224		43.72
00	33	ATOM	325	CA	SER I		4	-8.166	25.839	48.664 49.678		33.83
		ATOM	326	C	SER I		4	-7.495	24.557	50.117		42.10
		ATOM	327	0	SER I		4	-6.955	23.814	49.292		42.78
		ATOM	328	СВ	SER I		4	-9.576	25.530	49.226		28.60
	40	ATOM	329	OG	SER		4	-10.234	24.785	50.224		34.57
		ATOM	330	N	GLN .		15	-7.579	24.286	51.423		38.84
35		ATOM	331	CA	GLN I		15	-7.007	23.082	51.994		37.05
		ATOM	332	Č.	GLN .		15	-8.082	22.050	52.269		47.57
		ATOM	333	ō	GLN		15	-7.801	20.917	52.678		42.94
	45	ATOM	334	СВ	GLN .		15	-6.247	23.411	53.280		36.10
		ATOM	335	CG	GLN .		15	-5.246	24.539	53.034		54.73
		ATOM	336	CD	GLN .		15	-4.323	24.206	51.888		45.43
40		ATOM	337		GLN .		15	-4.257	24.888	50.833		39.23
40		ATOM	338	NE2	GLN .		15	-3.621	23.121	52.092		29.80
	50	ATOM	339	N	GLU .		16	-9.330	22.459	52.048		50.54
		ATOM	340	CA	GLU .		16	-10.454	21.573	52.283		50.99
		ATOM	341	С	GLU .		16	-11.496	21.583	51.179		54.49
		ATOM	342	0	GLU .		16	-11.518	22.406	50.261		54.00
		MOTA	343	CB	GLU .		16	-11.139	21.793	53.657	1.00	51.61
45	55	ATOM	344	ÇG	GLU .		16	-10.581	22.979	54.454		55.93
		ATOM	345	CD	GLU .		16	-11.427	23.329	55.646		78.67
		ATOM	346	OE1	GLU .	A 4	16	-12.563	23.765	55.543		69.56
		ATOM	347	OE2	GLU .	A 4	16	~10.814	23.129	56.796		75.10
		MOTA	348	N	ASP .		17	-12.387	20.630	51.300		48.90
	60	ATOM	349	CA	ASP .		17	-13.450	20.549	50.362		49.03
		MOTA	350	C	ASP .	A 4	17	-14.591	21.425	50.846		55.15
50		ATOM	351	0	ASP .	A 4	17	-14.760	21.631	52.044	1.00	56.66
		ATOM	352	CB	ASP .	A 4	17	-13,913	19.099	50.227	1.00	50.20
		ATOM	353	CG	ASP .	A 4	17	-13,083	18.376	49.218	1.00	66.88

5		ATOM	354	OD1	ASP A	47	-12.340	18.945	48.434	1.00 66.27
		ATOM	355		ASP A	47	-13.235	17.081	49.284	1.00 76.37
		ATOM	356	N	ASN A	48	-15.391	21.941	49.929	1.00 50.25
		ATOM	357	CA	ASN A	48	-16.519	22.755	50.339	1.00 48.45
	5	ATOM	358	С	ASN A	48	-16.115	24.000	51.115	1.00 43.07
		ATOM	359	0	ASN A	48	-16.699	24.351	52.138	1.00 39.78
		ATOM	360	CB	ASN A	48	-17.559	21.909	51.117	1.00 51.19
10		ATOM	361	CG	ASN A	48	-18.985	22.417	51.005	1.00 76.39
		ATOM	362		ASN A	48	-19.594	22.348	49.929	1.00 85.15
	10	ATOM	363		ASN A	48	-19.515	22.928	52.115	1.00 68.29
		ATOM	364	N	LEU A	49	-15.113	24.688	50.628	1.00 35.36
		ATOM	365	CA	LEU A	49	-14.728	25.874	51.335	1.00 34.40
		ATOM	366	c .	LEU A	49	-15.601	27.009	50.851	1.00 47.38
		ATOM	367	ŏ	LEU A	19	-15.421	27.515	49.734	1.00 45.47
15	15	ATOM	368	СВ	LEU A	49	-13.239	26.152	51.173	1.00 31.04
	10	ATOM	369	CG	LEU A	49	-12.781	27.394	51.885	1.00 29.82
		ATOM	370		LEU A	49	-12.725	27.137	53.385	1.00 28.15
		ATOM	371		LEU A	49	-11.394	27.753	51.368	1.00 30.24
						50	-16.568			
	20	MOTA	372	N	ARG A			27.363	51.699	1.00 50.49
	20	MOTA	373	CA	ARG A	50	-17.560	28.392	51.401	1.00 52.83
20		MOTA	374	C	ARG A	50	-17.169	29.838	51.702	1.00 55.57
		ATOM	375	0	ARG A	50	-17.627	30.760	51.011	1.00 53.89
		ATOM	376	CB	ARG A	50	-18.928	28.028	51.986	1.00 58.35
	25	ATOM	377	CG	ARG A	50	-19.863	27.354	50.980	1.00 74.76
	25	ATOM	378	CD	ARG A	50	-20.438	26.024	51.462	1.00 81.60
		ATOM	379	ΝE	ARG A	50	-21.214	25.355	50.415	1.00 94.37
		ATOM	380	CZ	ARG A	50	-22.465	24.888	50.538	1.00100.00
25 ·		ATOM	381	NH1	ARG A	50	-23.151	24.990	51.687	1.00100.00
		ATOM	382	NH2	ARG A	50	-23.046	24.297	49.471	1.00 74.34
	30	ATOM	383	N	SER A	51	-16.331	30.006	52.743	1.00 54.71
		ATOM	384	CA	SER A	51	-15.823	31.297	53.224	1.00 53.49
		ATOM	385	С	SER A	51	-14.495	31.156	53.955	1.00 53.57
		ATOM	386	0	SER A	51	-14.146	30.062	54.420	1.00 52.93
		ATOM	387	СВ	SER A	51	-16.788	31.900	54.232	1.00 54.03
30	35	ATOM	388	OG	SER A	51	-16.871	31.048	55.373	1.00 45.15
		ATOM	389	N	LEU A	52	-13.796	32.298	54.067	1.00 47.19
		ATOM	390	CA	LEU A	52	-12.519	32.422	54.762	1.00 45.66
		ATOM	391	С	LEU A	52	-12.415	33.671	55.640	1.00 50.43
		ATOM	392	ō	LEU A	52	-13.145	34.633	55.471	1.00 52.64
	40	ATOM	393	СВ	LEU A	52	-11.235	32.117	53.923	1.00 44.20
		ATOM	394	CG	LEU A	52	-10.896	33.044	52.745	1.00 43.98
35		ATOM	395		LEU A	52	-11.739	32.687	51.554	1.00 42.82
		ATOM	396		LEU A	52	-11.128	34.501	53.094	1.00 44.71
		ATOM	397	N	VAL A	53	-11.483	33.658	56.579	1.00 44.71
	45	ATOM	398	CA	VAL A	53	-11.271			
	43							34.781	57.455	1.00 41.69
		ATOM	399	C	VAL A	53	-9.859	35.309	57.339	1.00 44.25
		ATOM	400	0	VAL A	53	-8.866	34.551	57.302	1.00 45.42
40		ATOM	401	CB	VAL A	53	-11.565	34.420	58.906	1.00 45.48
	50	ATOM	402		VAL A	53	-11.223	35.554	59.853	1.00 44.94
	50	ATOM	403		VAL A	53	-13.030	34.073	59.050	1.00 45.79
		ATOM	404	N	LEU A	54	-9.796	36.627	57.166	1.00 35.12
		ATOM	405	CA	LEU A	54	-8.555	37.333	57.080	1.00 34.14
		ATOM	406	С	LEU A	54	-8.377	38.207	58.326	1.00 38.92
	مر س	ATOM	407	0	LEU A	54	-9.281	38.457	59.108	1.00 37.45
45	55	ATOM	408	CB	LEU A	54	-8.461	38.216	55.831	1.00 34.73
		ATOM	409	CG	LEU A	54	-8.539	37.469	54.510	1.00 40.25
		ATOM	410	CD1	LEU A	54	-8.416	38.488	53.374	1.00 40.69
		MOTA	411	CD2	LEU A	54	-7.424	36.428	54.415	1.00 39.64
		MOTA	412	N	ASP A	55	-7.192	38.674	58.524	1.00 35.02
	60	MOTA	413	CA	ASP A	55	-6.918	39.526	59.627	1.00 31.65
		ATOM	414	С	ASP A	55	-6.956	40.941	59.078	1.00 40.38
50		ATOM	415	0	ASP A	55	-6.754	41.151	57.886	1.00 39.98
		ATOM	416	СВ	ASP A	55	-5.494	39.232	60.075	1.00 30.92
		ATOM	417	CG	ASP A	55	-5.397	38.103	61.037	1.00 35.96
										2.22 00.00

5		ATOM	418	OD1	ASP A	55	-6.049	38.074	62.066	1.00 38.49
		ATOM	419		ASP A	55	-4.491	37.205	60.682	1.00 36.53
		ATOM	420	N	THR A		-7.196	41.900	59.963	1.00 42.93
		ATOM	421	CA	THR A		-7.243	43.334	59.661	1.00 41.75
	5	ATOM	422	С	THR A		-7.101	44.128	60.967	1.00 37.46
		ATOM	423	0	THR A		-7.517	43.687	62.049	1.00 36.98
		ATOM	424	CB	THR A		-8.514	43.825	58.894	1.00 37.17
10		MOTA	425	OG1	THR A		-9.587	43.957	59.805	1.00 31.84
		MOTA	426		THR A		-8.910	42.943	57.714	1.00 33.58
	10	MOTA	427	N	LYS A		-6.513	45.304	60.863	1.00 26.63
		ATOM	428	CA	LYS A		-6.363	46.134	62.020	1.00 25.64
		ATOM	429	С	LYS A		-6.585	47.539	61.547	1.00 30.08
		ATOM	430	0	LYS A	57	-5.854	48.012	60.711	1.00 25.68
4.5		ATOM	431	CB	LYS A	57	-4.991	45.983	62,641	1.00 27.34
15	15	MOTA	432	CG	LYS A	57	-4.907	46.387	64.100	1.00 35.83
		ATOM	433	CD	LYS A	57	-3.514	46.904	64.471	1.00 35.57
		MOTA	434	CE	LYS A	57	-2.901	46.225	65.689	1.00 50.54
		MOTA	435	NZ	LYS A	57	-2.521	47.180	66.757	1.00 55.43
		ATOM	436	N	ASP A	58	-7.617	48.188	62.065	1.00 32.68
	20	ATOM	437	CA	ASP A	58	-7.895	49.545	61.665	1.00 35.27
20		ATOM	438	С	ASP A	58	-7.894	49.710	60.149	1.00 38.24
20		ATOM	439	0	ASP A		-7.289	50.627	59.571	1.00 35.86
		ATOM	440	CB	ASP A		-6.968	50.550	62.386	1.00 37.22
		ATOM	441	CG	ASP A		-7.041	50.393	63.880	1.00 50.71
	25	ATOM	442	OD1	ASP A	58	-8.073	50.136	64.478	1.00 57.20
		ATOM	443	OD2	ASP A	58	-5.878	50.562	64.463	1.00 45.82
		MOTA	444	N	LEU A	59	-8.604	48.796	59.516	1.00 37.68
25		ATOM	445	CA	LEU A	59	-8.720	48.813	58.079	1.00 39.36
		MOTA	446	С	LEU A	59	-10.077	49.243	57.555	1.00 45.51
	30	MOTA	447	0	LEU A	59	-11.146	48.946	58.120	1.00 44.18
		ATOM	448	CB	LEU A	59	-8.265	47.506	57.422	1.00 38.42
		ATOM	449	CG	LEU A	59	-6.762	47.475	57.218	1.00 37.40
		ATOM	450	CD1	LEU A	59	-6.392	46.173	56.526	1.00 36.39
		ATOM	451	CD2	LEU A	59	-6.321	48.655	56.361	1.00 36.57
30	35	MOTA	452	N	THR A	60	-9.984	49.949	56.437	1.00 42.59
		ATOM	453	CA	THR A	60	-11.132	50.483	55.734	1.00 42.63
		ATOM	454	С	THR A	60	-11.357	49.705	54.463	1.00 38.18
		MOTA	455	0	THR A	60	-10.632	49.856	53.454	1.00 34.33
		MOTA	456	CB	THR A	60	-11.030	52.028	55.532	1.00 65.15
	40	ATOM	457	OG1	THR A	60	-11.806	52.736	56.504	1.00 67.56
25		MOTA	458	CG2	THR A	60	-11.345	52.480	54.104	1.00 56.89
35		ATOM	459	N	ILE A	61	-12.360	48.847	54.571	1.00 33.39
		ATOM	460	CA	ILE A	61	-12.753	47.975	53.482	1.00 35.89
		MOTA	461	С	ILE A	61	-13.726	48.634	52.533	1.00 41.05
	45	MOTA	462	0	ILE A	61	-14.913	48.706	52.840	1.00 40.08
		MOTA	463	СВ	ILE A	61	-13.403	46.670	53.944	1.00 39.71
		MOTA	464		ILE A		-12.482	45.826	54.832	1.00 39.90
40		MOTA	465		ILE A		-13.788	45.900	52.691	1.00 38.96
,,,	**	MOTA	466	CD1	ILE A	61	-11.027	45.851	54.358	1.00 49.61
	50	MOTA	467	N	GLU A		-13.219	49.080	51.391	1.00 40.23
		ATOM	468	CA	GLU A		-14.040	49.700	50.365	1.00 41.73
		ATOM	469	С	GLU A		-14.986	48.633	49.826	1.00 47.09
		ATOM	470	0	GLU A		-16.207	48.726	49.926	1.00 47.52
	E E	MOTA	471	CB	GLU A		-13.138	50.272	49.239	1.00 44.08
45	55	ATOM	472	CG	GLU A		-13.765	51.406	48.381	1.00 64.08
		MOTA	473	CD	GLU A		-14.686	50.946	47.256	1.00100.00
		ATOM	474		GLU A		-15.458	50.002	47.376	1.00100.00
		ATOM	475		GLU A		-14.591	51.670	46.146	1.00 75.11
	60	MOTA	476	N	LYS A		-14.399	47.580	49.267	1.00 43.46
	60	MOTA	477	CA	LYS A		-15.168	46.474	48.746	1.00 40.53
		ATOM	478	С	LYS A		-14.250	45.307	48.489	1.00 45.38
50		MOTA	479	0	LYS A		-13.046	45.500	48.362	1.00 43.51
		ATOM	480	CB	LYS A		-15.818	46.830	47.428	1.00 40.46
		MOTA	481	CG	LYS A	63	14.789	46.959	46.321	1.00 20.53

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5		ATOM	482	CD	LYS	Α	63	-15.367	47.555	45.054	1.00 28.36
		ATOM	483	CE	LYS		63	-14.315	48.158	44.139	1.00 40.61
		ATOM	484	NZ	LYS		63	-14.588	47.938	42.711	1.00 54.71
		ATOM	485	N	VAL	A	64	-14.862	44.116	48.441	1.00 45.57
	5	ATOM	486	CA	VAL	Α	64	-14.190	42.844	48.171	1.00 44.90
		ATOM	487	С	VAL	Α	64	-14.666	42.263	46.841	1.00 46.44
		MOTA	488	0	VAL	Α	64	-15.826	41.917	46.700	1.00 45.81
10		ATOM	489	CB	VAL	Α	64	-14.505	41.748	49.192	1.00 46.24
		MOTA	490	CG1	VAL	Α	64	-13.864	40.471	48.669	1.00 44.81
	10	ATOM	491	CG2	VAL	А	64	-14.040	42.048	50.627	1.00 44.77
		MOTA	492	N	VAL		65	-13.793	42.099	45.875	1.00 43.10
		ATOM	493	CA	VAL		65	-14.240	41.537	44.604	1.00 41.42
		ATOM	494	С	VAL		65	-13.707	40.156	44.282	1.00 42.13
15	1.5	ATOM	495	0	VAL		65	-12.605	39.787	44.660	1.00 42.64
7.5	15	MOTA	496	CB	VAL		65	-13.856	42.462	43.484	1.00 44.58
		ATOM	497		VAL		65	-14.520	42.037	42.189	1.00 42.79
		ATOM	498		VAL		65	-14.264	43.874	43.883	1.00 45.05
		MOTA	499	N	ILE		66	-14.515	39.402	43.556	1.00 38.68
	20	MOTA	500	CA	ILE		66	-14.179	38.053	43.113	1.00 39.98
	20	MOTA	501	C	ILE		66	-14.899	37.774	41.802	1.00 44.86
20		ATOM	502	0	ILE		66	-16.136	37.735	41.729	1.00 42.69
		ATOM	503	CB	ILE		66	-14.520	36.947	44.113	1.00 44.28
		MOTA	504		ILE		66	-13.813	37.127	45.445	1.00 47.27
	25	ATOM	505		ILE		66 66	-14.141 -14.352	35.578	43.550	1.00 42.84
	23	ATOM	506 507		ILE		66 67	-14.332	36.169	46.514	1.00 38.79
		ATOM ATOM	508	N CA	ASN ASN		67	-14.715	37.549 37.266	40.759	1.00 42.94
05		ATOM	509	C	ASN		67	-15.541	38.444	39.472 39.008	1.00 44.24 1.00 54.25
25		ATOM	510	ŏ	ASN		67	-16.743	38.344	38.768	1.00 57.56
	30	ATOM	511	СВ	ASN		67	-15.595	36.007	39.507	1.00 37.30
	50	ATOM	512	CG	ASN		67	-14.788	34.759	39.745	1.00 57.39
		ATOM	513		ASN		67	-13.581	34.711	39.454	1.00 52.63
		ATOM	514		ASN		67	-15.446	33.760	40.317	1.00 44.54
		ATOM	515	N	GLY		68	-14.876	39.574	38.899	1.00 50.43
30	35	ATOM	516	CA	GLY		68	-15.517	40.796	38.462	1.00 48.89
		ATOM	517	C	GLY		68	-16.807	41.115	39.194	1.00 48.77
		ATOM	518	0	GLY		68	-17.523	42.018	38.803	1.00 51.39
		ATOM	519	N	GLN		69	-17.129	40.385	40.244	1.00 40.06
		ATOM	520	CA	GLN	Α	69	-18.348	40.716	40.928	1.00 40.02
	40	ATOM	521	C	GLN	Α	69	-18.031	41.059	42.364	1.00 50.45
		ATOM	522	0	GLN	Α	69	-16.943	40.748	42.855	1.00 50.53
35		ATOM	523	CB	GLN	А	69	-19.415	39.602	40.829	1.00 40.78
		ATOM	524	CG	GLN	Α	69	-19.966	39.367	39.414	1.00 23.77
		ATOM	525	CD	GLN	Α	69	-20.513	40.646	38.831	1.00 56.53
	45	MOTA	526	OE1	GLN	Α	69	-19.974	41.198	37.859	1.00 55.28
		ATOM	527	NE2	GLN	Α	69	-21.588	41.134	39.437	1.00 62.26
		ATOM	528	N	GLU	А	70	-18.975	41.718	43.028	1.00 49.43
40		ATOM	529	CA	GLU		70	-18.766	42.094	44.407	1.00 50.67
	60	ATOM	530	С	GLU		70	-19.296	40.996	45.288	1.00 57.90
	50	ATOM	531	0	GLU		70	-20.272	40.367	44.909	1.00 63.90
		MOTA	532	СВ	GLU		70	-19.449	43.434	44.732	1.00 52.26
		ATOM	533	CG	GLU		70	-18.824	44.624	43.970	1.00 64.80
		ATOM	534	CD	GLU		70	-19.181	45.967	44.555	1.00 91.82
	<i></i>	ATOM	535		GLU		70	-19.749	46.108	45.629	1.00100.00
45	55	MOTA	536		GLU		70	-18.814	46.963	43.785	1.00 76.01
		ATOM	537	N	VAL		71.	-18.655	40.742	46.433	1.00 47.28
		ATOM	538	CA	VAL		71	-19.119	39.685	47.335	1.00 43.84
		ATOM	539	C	VAL		71	-19.434	40.153	48.768	1.00 41.62
	60	ATOM	540	0	VAL		71	-18.983	41.206	49.254	1.00 35.70
	oo	ATOM	541	CB	VAL		71	-18.308	38.361	47.273	1.00 46.05
50		ATOM	542		VAL		71	-18.062	37.923	45.827	1.00 45.19
50		ATOM	543		VAL		71	-16.979 -20.339	38.460	48.017	1.00 45.24
		ATOM	544	N	LYS		72	-20.239	39.343	49.431	1.00 39.34
		MOTA	545	CA	LYS	А	72	-20.610	39.594	50.792	1.00 42.40

5		MOTA	546	С	LYS A	72	-19.347	39.466	51.668	1.00 56.92
		MOTA	547	0	LYS A	72	-18.399	38.729	51.334	1.00 59.27
		MOTA	548	CB	LYS A	72	-21.719	38.629	51.211	1.00 45.76
		ATOM	549	CG	LYS A	72	-22.378	38.960	52.557	1.00 86.98
	5	MOTA	550	CD	LYS A	72	-23.898	38.767	52.606	1.00100.00
		ATOM	551	CE	LYS A	72	-24.656	40.012	53.077	1.00100.00
		ATOM	552	NZ	LYS A	72	-26.011	39.730	53.592	1.00100.00
10		ATOM	553	N	TYR A	73	-19.332	40.210	52.780	1.00 55.45
		ATOM	554	CA	TYR A	73	-18.236	40.226	53.747	1.00 53.31
	10	ATOM	555	c .	TYR A	73	-18.636	40.884	55.068	1.00 50.87
	••	MOTA	556	ō	TYR A	73	-19.552	41.703	55.139	1.00 47.82
		MOTA	557	СВ	TYR A	73	-16.891	40.741	53.214	
		MOTA	558	CG	TYR A	73	-16.765	42.244	53.227	1.00 52.73 1.00 51.76
		ATOM	559		TYR A	73				
15	15	ATOM	560				- <u>1</u> 6.539	42.946	54.416	1.00 52.82
	13				TYR A	73	-16.927	42.967	52.039	1.00 53.30
		MOTA	561		TYR A	73	-16.439	44.340	54.422	1.00 52.71
		MOTA	562		TYR A	73	-16.804	44.359	52.026	1.00 55.39
		MOTA	563	CZ	TYR A	73	-16.592	45.044	53.229	1.00 63.45
	20	MOTA	564	OH	TYR A	73	-16.471	46.404	53.215	1.00 69.53
	20	MOTA	565	N	ALA A	74	-17.927	40.494	56.112	1.00 45.37
20		MOTA	566	CA	ALA A	74	-18.180	40.999	57.433	1.00 42.62
		MOTA	567	С	ALA A	74	-16.892	41.265	58.222	1.00 47.81
		MOTA	568	0	ALA A	74	-15.894	40.554	58.133	1.00 45.50
		MOTA	569	CB	ALA A	74	-19.111	40.035	58.170	1.00 40.75
	25	ATOM	570	N	LEU A	75	-16.930	42.323	59.005	1.00 49.02
		ATOM	571	CA	LEU A	75	-15.829	42.693	59.869	1.00 48.85
		MOTA	572	С	LEU A	75	-16.319	42.464	61.281	1.00 47.18
25		ATOM	573	0	LEU A	75	-17.309	43.021	61.687	1.00 44.35
		ATOM	574	СВ	LEU A	75	-15.332	44.136	59.675	1.00 49.64
	30	ATOM	575	CG	LEU A	75	-14.789	44.357	58.270	1.00 58.09
		ATOM	576		LEU A	75	-14.524	45.841	58.023	1.00 61.34
		ATOM	577		LEU A	75	-13.512	43.565	58.069	1.00 62.34
		ATOM	578	N	GLY A	76	-15.647	41.592	62.004	1.00 47.67
		ATOM	579	CA	GLY A	76	-16.034	41.281	63.359	1.00 46.79
30	35	ATOM	580	c.	GLY A	76	-15.495	42.337	64.279	1.00 47.74
50	<i>55</i>	ATOM	581	ŏ	GLY A	76	-14.656	43.171	63.882	1.00 47.74
		ATOM	582	N	GLU A	77	-15.988	42.311	65.502	1.00 42.87
		ATOM	583	CA	GLU A	77	-15.526	43.300		
		ATOM	584	C	GLU A	77			66.431	1.00 52.14
	40						-14.029	43.195	66.679	1.00 56.71
	40	MOTA	585	0	GLU A	77	-13.418	42.120	66.591	1.00 55.78
35		ATOM	586	CB	GLU A	77	-16.357	43.341	67.732	1.00 55.55
-		ATOM	587	CG	GLU A	77	-17.198	42.063	67.969	1.00 79.57
		ATOM	588	CD	GLU A	77	-17.440	41.739	69.427	1.00100.00
	45	ATOM	589		GLU A	77	-16.537	41.435	70.211	1.00100.00
	45	ATOM	590		GLU A	77	-18.712	41.799	69.770	1.00100.00
		ATOM	591	N	ARG A	78	-13.452	44.344	67.000	1.00 54.17
		ATOM	592	CA	ARG A	78	-12.041	44.433	67.298	1.00 53.38
40		ATOM	593	С	ARG A	78	-11.627	43.656	68.579	1.00 58.88
70	• •	ATOM	594	0	ARG A	78	-12.247	43.767	69.635	1.00 61.35
	50	ATOM	595	CB	ARG A	78	-11.571	45.891	67.367	1.00 41.96
		ATOM	596	CG	ARG A	78	-10.050	46.006	67.326	1.00 38.20
		ATOM	597	CD	ARG A	78	-9.537	47.411	67.551	1.00 44.73
		ATOM	598	NE	ARG A	78	-8.294	47.648	66.842	1.00 66.47
	•	ATOM	599	CZ	ARG A	78	-7.250	48.247	67.389	1.00 97.61
45	55	ATOM	600		ARG A	78	-7.276	48.692	68.645	1.00100.00
40		ATOM	601		ARG A	78	-6.151	48.413	66.663	1.00 80.10
		ATOM	602	N	GLN A	79	-10.557	42.857	68.463	1.00 49.54
		ATOM	603	CA	GLN A	79	-9.995	42.115	69.566	1.00 49.34
		ATOM	604	C	GLN A	79	-8.664			
	60	ATOM	605	Ö			-7.626	42.789	69.865	1.00 49.77
	00	ATOM	606		GLN A	79		42.421	69.333	1.00 52.63
E0				CB	GLN A	79	-9.803	40.613	69.240	1.00 49.05
50		ATOM	607	CG	GLN A	79	-11.109	39.794	69.339	1.00 57.32
		ATOM	608	CD	GLN A	79	-11.043	38.435	68.656	1.00 69.51
		ATOM	609	OEl	GLN A	79	-10.400	37.480	69.152	1.00 49.72

5		MOTA	610	NE2	GLN	А	79	-11.727	38.340	67.517	1.00 62.60
		ATOM	611	N	SER		80	-8.699	43.826	70.683	1.00 41.74
		ATOM	612	CA	SER	А	80	-7.490	44.543	71.022	1.00 37.90
	_	ATOM	613	С	SER	Α	80	-6.437	44.559	69.920	1.00 35.98
	5	ATOM	614	0	SER	А	80	-6.736	44.939	68.801	1.00 34.52
		ATOM	615	CB	SER	А	80	-6.910	44.144	72.372	1.00 39.07
		MOTA	616	OG	SER	А	80	-7.255	42.803	72.684	1.00 61.32
10		ATOM	617	N	TYR	A	81	-5.206	44.154	70.289	1.00 29.92
		ATOM	618	CA	TYR	А	81	-4.027	44.114	69.430	1.00 26.45
	10	ATOM	619	С	TYR	Α	81	-4.163	43.116	68.285	1.00 30.82
		ATOM	620	0	TYR	Α	81	-3.480	43.215	67.269	1.00 34.48
		ATOM	621	CB	TYR		81	-2.727	43.893	70.257	1.00 25.19
		ATOM	622	CG	TYR		81	-2.713	42.491	70.839	1.00 24.57
15	1.6	ATOM	623		TYR		81	-3.327	42.247	72.066	1.00 27.27
15	15	ATOM	624		TYR		81	-2.165	41.410	70.148	1.00 21.82
		ATOM	625		TYR		81	-3.380	40.975	72.632	1.00 26.49
		ATOM	626		TYR		81	-2.230	40.122	70.682	1.00 23.48
		ATOM	627	CZ	TYR		81	-2.827	39.908	71.930	1.00 38.28
	20	ATOM	628	ОН	TYR		81	-2.889	38.653	72.493	1.00 42.17
	20	ATOM	629	N	LYS		82	-5.038	42.136	68.415	1.00 26.97
20		ATOM	630	CA	LYS		82	-5.170	41.229	67.293	1.00 27.99
		ATOM	631	C	LYS		82	-5.867	41.898	66.072	1.00 38.90
		ATOM	632	0	LYS		82	-5.614	41.541	64.900	1.00 37.15
	25	MOTA	633	CB	LYS		82	-5.785	39.918	67.708	1.00 27.59
	23	ATOM	634	CG	LYS		82	-5.169	39.451	69.008	1.00 39.68
		ATOM	635	CD	LYS		82	-5.435	37.993	69.350	1.00 46.78
		ATOM ATOM	636	CE	LYS		82	-6.414	37.819	70.492	1.00 59.84
25		ATOM	637 638	NZ N	LYS		82	-7.097	36.523	70.452	1.00 63.48
	30	ATOM	639	CA	GLY		83 83	-6.738	42.894	66.367	1.00 35.64
	50	ATOM	640	c	GLY		83	-7.512 -9.966	43.620	65.368	1.00 33.65
		ATOM	641	ŏ	GLY		83	-8.866 -9.297	42.925 42.063	65.111	1.00 32.95
		ATOM	642	N	SER		84	-9.535	43.300	65.870 64.026	1.00 28.28
		ATOM	643	CA	SER		84	-10.839	42.742	63.673	1.00 34.51 1.00 36.13
30	35	ATOM	644	C	SER		84	-10.796	41.724	62.549	1.00 40.65
		ATOM	645	ō	SER		84	-10.173	41.893	61.501	1.00 39.77
		ATOM	646	СВ	SER		84	-11.883	43.808	63.383	1.00 37.68
		ATOM	647	ŌĞ	SER		84	-11.812	44.832	64.352	1.00 45.14
		ATOM	648	N	PRO		85	-11.491	40.656	62.791	1.00 37.01
	40	ATOM	649	CA	PRO		85	-11.573	39.559	61.863	1.00 34.91
		MOTA	650	С	PRO		85	-12.459	39.946	60.712	1.00 35.92
35		ATOM	651	0	PRO	Α	85	-13.514	40.522	60.941	1.00 35.30
		ATOM	652	CB	PRO		85	-12.227	38.406	62.647	1.00 37.00
		ATOM	653	CG	PRO	Α	85	-12.714	38.981	63.974	1.00 44.97
	45	ATOM	654	CD	PRO	Α	85	-12.325	40.462	64.004	1.00 40.72
		ATOM	655	N	MET	А	86	-12.018	39.642	59.487	1.00 30.47
		ATOM	656	CA	MET	Α	86	-12.756	39.960	58.275	1.00 28.55
40		ATOM	657	С	MET	Α	86	-13.165	38.683	57.552	1.00 40.49
40		MOTA	658	0	MET	A	86	-12.338	38.015	56.954	1.00 39.69
	50	ATOM	659	CB	MET	Α	86	-11.921	40.829	57.337	1.00 29.51
		ATOM	660	CG	MET	А	86	-12.750	41.242	56.136	1.00 37.40
		ATOM	661	SD	MET		86	-11.816	41.878	54.701	1.00 47.84
		ATOM	662	CE	MET	Α	86	-13.244	42.527	53.805	1.00 46.52
		ATOM	663	N	GLU	Α	87	-14.441	38.324	57.610	1.00 44.34
45	55	ATOM	664	CA	GLU	A	87	-14.912	37.107	56.950	1.00 47.21
		MOTA	665	С	GLU		87	-15.495	37.352	55.560	1.00 51.53
		ATOM	666	0	GLU		87	-16.425	38.129	55.424	1.00 53.92
		ATOM	667	СВ	GLU		87	-15.942	36.390	57.813	1.00 49.46
	60	ATOM	668	CG	GLU		87	-16.144	34.937	57.389	1.00 56.39
	60	ATOM	669	CD	GLU		87	-17.300	34.316	58.104	1.00 80.78
	7	ATOM	670		GLU		87	-18.439	34.738	57.994	1.00 86.69
50		ATOM	671		GLU		87	-16.943	33.301	58.868	1.00 68.69
		ATOM	672	N	ILE		88	-14.942	36.659	54.544	1.00 43.84
		ATOM	673	CA	ILE	A	88	-15.332	36.765	53.145	1.00 40.15

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5		ATOM	674	С	ILE A	88	-16.145	35.610	52.613	1.00 46.72
•		ATOM	675	ò	ILE A	88	-15.725	34.460	52.656	1.00 48.10
		ATOM	676	СB	ILE A	88	-14.107	36.891	52.292	1.00 39.13
		ATOM	677		ILE A	88	-13.328	38.146	52.696	1.00 38.40
	5	ATOM	678		ILE A	88	-14.538	36.932	50.839	1.00 28.13
	•	ATOM	679		ILE A	88	-11.944	38.200	52.051	1.00 30.07
		ATOM	680	N	SER A	89	-17.314	35.931	52.077	1.00 45.16
10		ATOM	681	CA	SER A	89	-18.181	34.893	51.559	1.00 44.76
		ATOM	682	c .	SER A	89	-17.902	34.531	50.131	1.00 46.01
	10	ATOM	683	0	SER A	89	-18.048	35.347	49.243	1.00 44.34
		ATOM	684	СВ	SER A	89	-19.657	35.121	51.827	1.00 51.87
		ATOM	685	OG	SER A	89	-19.942	34.834	53.198	1.00 69.07
		ATOM	686	N	LEU A	90	-17.494	33.279	49.914	1.00 46.43
		ATOM	687	CA	LEU A	90	-17.204	32.804	48.575	1.00 46.93
15	15	ATOM	688	C	LEU A	90	-18.450	32.235	47.935	1.00 55.26
		ATOM	689	Ó	LEU A	90	-19.210	31.476	48.556	1.00 54.94
		ATOM	690	СВ	LEU A	90	-16.080	31.750	48.521	1.00 46.14
		ATOM	691	CG	LEU A	90	-15.262	31.607	49.792	1.00 50.78
		ATOM	692		LEU A	90	-14.546	30.261	49.806	1.00 50.27
	20	ATOM	693		LEU A	90	-14.219	32.708	49.863	1.00 55.52
		ATOM	694	N	PRO A	91	-18.626	32.607	46.683	1.00 54.81
20		ATOM	695	CA	PRO A	91	-19.756	32.183	45.870	1.00 58.45
		ATOM	696	c	PRO A	91	-19.585	30.782	45.254	1.00 67.78
		ATOM	697	ō	PRO A	91	-20.500	30.250	44.623	1.00 68.64
	25	ATOM	698	СВ	PRO A	91	-19.843	33.213	44.738	1.00 59.70
		ATOM	699	CG	PRO A	91	-18.503	33.952	44.711	1.00 61.25
		ATOM	700	CD	PRO A	91	-17.731	33.539	45.961	1.00 54.16
25		ATOM	701	N	ILE A	92	-18.413	30.177	45.416	1.00 64.82
23		ATOM	702	CA	ILE A	92	-18.210	28.863	44.850	1.00 65.03
	30	ATOM	703	C	ILE A	92	-17.485	27.948	45.801	1.00 66.34
		ATOM	704	0	ILE A	92	-16.258	27.984	45.865	1.00 70.20
		ATOM	705	СB	ILE A	92	-17.433	28.927	43.547	1.00 69.56
		ATOM	706		ILE A	92	-18.298	29.495	42.430	1.00 70.02
		MOTA	707		ILE A	92	-16.975	27.517	43.171	1.00 71.86
30	35	ATOM	708		ILE A	92	-17.528	29.672	41.121	1.00 80.63
		ATOM	709	N	ALA A	93	-18.219	27.115	46.534	1.00 54.40
		ATOM	710	CA	ALA A	93	-17.526	26.247	47.452	1.00 51.74
		ATOM	711	С	ALA A	93	-16.265	25.750	46.804	1.00 52.66
		ATOM	712	0	ALA A	93	-16.288	25.319	45.662	1.00 49.87
	40	MOTA	713	CB	ALA A	93	-18.367	25.101	47.968	1.00 .52.76
		MOTA	714	N	LEU A	94	-15.162	25.861	47.544	1.00 48.18
35		ATOM	715	CA	LEU A	94	-13.862	25.425	47.067	1.00 43.27
		MOTA	716	С	LEU A	94	-13.566	24.066	47.581	1.00 43.98
		ATOM	717	0	LEU A	94	-14.086	23.633	48.601	1.00 44.63
	45	ATOM	718	СВ	LEU A	94	-12.713	26.344	47.509	1.00 41.05
		ATOM	719	CG	LEU A	94	-12.685	27.638	46.739	1.00 40.03
		ATOM	720	CD1	LEU A	94	-11.272	28.200	46.751	1.00 36.88
40		ATOM	721		LEU A	94	-13.115	27.343	45.311	1.00 44.98
40		ATOM	722	N	SER A	95	-12.706	23.406	46.875	1.00 43.26
	50	ATOM	723	CA	SER A	95	-12.321	22.074	47.256	1.00 43.76
		ATOM	724	С	SER A	95	-10.807	21.991	47.344	1.00 38.58
		MOTA	725	0	SER A	95	-10.087	22.944	46.975	1.00 36.78
		MOTA	726	СВ	SER A	95	-12.902	21.092	46.256	1.00 51.55
		ATOM	727	OG	SER A	95	-14.299	21.305	46.156	1.00 62.74
45	55	ATOM	728	N	LYS A	96	-10.321	20.863	47.830	1.00 31.10
70		ATOM	729	CA	LYS A	96	-8.883	20.723	47.958	1.00 34.92
		ATOM	730	С	LYS A	96	-8.058	21.238	46.777	1.00 45.63
		ATOM	731	o	LYS A	96	-8.400	21.063	45.612	1.00 49.35
		ATOM	732	СВ	LYS A	96	-8.401	19.366	48.451	1.00 38.53
	60	MOTA	733	CG	LYS A	96	-9.189	18.871	49.651	1.00 68.97
		ATOM	734	CD	LYS A	96	-8.691	17.549	50.221	1.00 80.86
50		ATOM	735	CE	LYS A	96	-9.596	17.011	51.330	1.00 92.53
		ATOM	736	NZ	LYS A	96	-9.049	15.833	52.029	1.00100.00
		ATOM	737	N	ASN A	97	-6.944	21.873	47.108	1.00 41.92

5		ATOM	738	CA	ASN A		-6.009	22.403	46.139	1.00 40.91
		ATOM	739	С	ASN A		-6.606	23.348	45.088	1.00 42.64
		ATOM	740	0	asn a		-5.963	23.681	44.068	1.00 38.69
	_	ATOM	741	СВ	ASN A		-5.084	21.304	45.583	1.00 28.16
	5	ATOM	742	CG	ASN A		-4.327	20.568	46.677	1.00 52.21
		ATOM	743		asn a		-3.089	20.627	46.744	1.00 55.30
		ATOM	744	ND2	ASN A	. 97	-5.060	19.858	47.533	1.00 53.87
10		ATOM	745	N	GLN A	. 98	-7.833	23.791	45.382	1.00 36.59
		ATOM	746	CA	GLN A	. 98	-8.557	24.718	44.536	1.00 38.44
	10	ATOM	747	С	GLN A	. 98	-8.288	26.181	44.951	1.00 43.30
		MOTA	748	0	GLN A	98	-8.248	26.526	46.138	1.00 43.40
		MOTA	749	CB	GLN A	98	-10.064	24.395	44.575	1.00 42.26
		ATOM	750	CG	GLN A	. 98	-10.553	23.538	43.385	1.00 68.24
		ATOM	751	CD	GLN A	. 98	-12.008	23.778	43.010	1.00 95.57
15	15	ATOM	752	OE1	GLN A	. 98	-12.890	22.935	43.278	1.00 86.92
		ATOM	753	NE2	GLN A	. 98	-12.271	24.935	42.393	1.00 95.48
		ATOM	754	N	GLU A		-8.089	27.062	43.973	1.00 39.70
		ATOM	755	CA	GLU A		-7.817	28.468	44.280	1.00 40.49
		ATOM	756	c	GLU A		-8.750	29.536	43.683	1.00 47.84
	20	ATOM	757	ō	GLU A		-9.330	29.394	42.606	1.00 47.84
		ATOM	758	СВ	GLU A		-6.361	28.866	43.951	1.00 40.24
20		ATOM	759	CG	GLU A		-5.608	27.861		
		ATOM	760	CD	GLU A		-4.120	28.119	43.080	1.00 44.16
	•	ATOM	761		GLU A		-3.636	29.062	42.990	1.00 65.64
	25	ATOM	762	OE2					42.376	1.00 73.95
	23	ATOM					-3.395	27.210	43.614	1.00 55.99
			763	N	ILE A		-8.848	30.643	44.418	1.00 43.55
		ATOM	764	CA	ILE A		-9.595	31.800	44.005	1.00 43.46
25		ATOM	765	C	ILE A		-8.701	32.992	44.238	1.00 53.31
	30	ATOM	766	0	ILE A		-7.725	32.927	45.004	1.00 55.16
	30	ATOM	767	CB	ILE A		-10.881	32.068	44.773	1.00 46.65
		ATOM	768		ILE A		-10.762	31.640	46.227	1.00 50.76
		ATOM	769		ILE A		-12.111	31.486	44.106	1.00 46.76
		ATOM	770		ILE A		-9.959	32.620	47.087	1.00 64.36
	25	ATOM	771	N	VAL A		-9.060	34.076	43.580	1.00 48.20
30	35	ATOM	772	CA	VAL A		-8.382	35.329	43.760	1.00 45.63
		ATOM	773	С	VAL A		-9.383	36.351	44.295	1.00 48.59
		ATOM	774	0	VAL A		-10.331	36.722	43.623	1.00 51.29
		ATOM	775	CB	VAL A	101	-7.461	35.793	42.633	1.00 45.06
	40	ATOM	776		VAL A		-7.693	35.000	41.378	1.00 43.25
	40	ATOM	777	CG2	VAL A	101	-7.609	37.289	42.395	1.00 45.02
Δ.		ATOM	778	N	ILE A	. 102	-9.182	36.738	45.546	1.00 41.15
35		ATOM	779	CA	ILE A	102	-10.023	37.690	46.238	1.00 39.43
		ATOM	780	С	ILE A	102	-9.439	39.062	46.170	1.00 49.35
		ATOM	781	0	ILE A	102	-8.331	39.274	46.659	1.00 53.80
	45	ATOM	782	CB	ILE A	102	-10.097	37.319	47.694	1.00 39.19
		MOTA	783	CG1	ILE A	102	-10.180	35.800	47.809	1.00 35.28
		ATOM	784	CG2	ILE A	102	-11.300	37.992	48.341	1.00 35.25
40		MOTA	785		ILE A		-10.962	35.392	49.044	1.00 47.09
40		MOTA	786	N	GLU A	103	-10.192	39.984	45.572	1.00 43.20
	50	ATOM	787	CA	GLU A		-9.748	41.362	45.433	1.00 39.88
		ATOM	788	С	GLU A		-10.378	42.299	46.425	1.00 44.03
		MOTA	789	0	GLU A		-11.580	42.558	46.385	1.00 41.34
		ATOM	790	СВ	GLU A		-9.950	41.930	44.047	1.00 39.11
		ATOM	791	CG	GLU A		-9.017	43.112	43.863	1.00 35.11
	55	ATOM	792	CD	GLU A		-9.150	43.666		
45	55	ATOM	793		GLU A		-10.157		42.485	1.00 61.93
		ATOM	794		GLU A			44.234	42.100	1.00 69.89
							-8.087	43.457	41.744	1.00 76.18
		ATOM	795	N	ILE A		-9.534	42.797	47.322	1.00 42.69
	60	ATOM	796	CA	ILE A		-9.969	43.718	48.346	1.00 40.72
	00	ATOM	797	C	ILE A		-9.522	45.167	48.099	1.00 46.21
		ATOM	798	0	ILE A		-8.346	45.478	47.866	1.00 42.68
50		ATOM	799	CB	ILE A		-9.578	43.283	49.754	1.00 41.75
		· ATOM	800		ILE A		-10.006	41.855	50.032	1.00 39.85
		ATOM	801	CG2	ILE A	104	-10.225	44.222	50.768	1.00 41.53

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5		ATOM	802		ILE			-8.839	40.995	50.485	1.00 34.17
		MOTA	803	N	SER			-10.506	46.056	48.173	1.00 47.94
		MOTA	804	CA	SER			-10.278	47.481	48.046	1.00 48.05
•	5	ATOM	805	C	SER			-10.184	47.977	49.482	1.00 42.39
	,	MOTA	806	0	SER			-11.134	47.879	50.263	1.00 39.69
		ATOM ATOM	807	CB	SER.			-11.399	48.180	47.290	1.00 53.77
10		ATOM	808 809	og N	SER.			-11.399	47.789	45.930	1.00 60.69
70		ATOM	810	CA	PHE PHE			-9.020	48.445	49.857	1.00 35.07
	10	ATOM	811	C	PHE .			-8.844 -8.177	48.890 50.238	51.223 51.262	1.00 34.98
		ATOM	812	ŏ	PHE			-7.607	50.730	50.265	1.00 39.26 1.00 34.24
		ATOM	813	СВ	PHE			-8.015	47.864	52.060	1.00 34.24
		ATOM	814	ĊĠ	PHE			-6.581	47.815	51.556	1.00 37.24
		ATOM	815		PHE			-6.251	47.073	50.422	1.00 39.71
15	15	ATOM	816		PHE .			-5.579	48.579	52.161	1.00 36.44
		ATOM	817	CEl	PHE .	A]	106	-4.950	47.086	49.920	1.00 41.48
		ATOM	818	CE2	PHE .	A 1	106	-4.273	48.609	51.672	1.00 38.19
		ATOM	819	CZ	PHE .	A 1	106	-3.961	47.856	50.540	1.00 37.91
	••	ATOM	820	N	GLU .	A 1	107	-8.284	50.794	52.453	1.00 40.64
	20	ATOM	821	CA	GLU .			-7.711	52.064	52.848	1.00 43.81
20		ATOM	B22	С	GLU .			-7.206	51.869	54.284	1.00 43.82
		ATOM	823	0	GLU .			-7.933	51.303	55.121	1.00 38.38
		ATOM	824	CB	GLU .			-8.737	53.234	52.753	1.00 46.93
	25	ATOM	825	CG	GLU .			-8.107	54.637	52.467	1.00 67.21
	25	ATOM	826	CD	GLU .			-9.086	55.715	52.042	1.00100.00
		ATOM	827		GLU .			-10.208	55.504	51.599	1.00100.00
		ATOM	828		GLU .			-8.631	56.938	52.221	1.00 93.72
25		ATOM ATOM	829 830	N CA	THR .			-5.963	52.294	54.551	1.00 39.12
	30	ATOM	831	C	THR.			-5.345	52.175	55.873	1.00 39.69
	50	ATOM	832	0	THR.			-5.564 -5.565	53.427 54.552	56.724	1.00 49.82
		ATOM	833	СВ	THR .			-3.810	52.095	56.177 55.722	1.00 50.94 1.00 40.40
		ATOM	834		THR .			-3.360	53.226	54.981	1.00 40.40
		ATOM	835		THR			-3.371	50.802	55.042	1.00 46.43
30	35	ATOM	836	N	SER .			-5.698	53.217	58.065	1.00 42.02
••		ATOM	837	CA	SER .			-5.848	54.294	59.038	1.00 38.13
•		ATOM	838	С	SER .			-4.555	55.101	59.082	1.00 38.47
		ATOM	839	0	SER .	A 1	109	-3.460	54.583	58.921	1.00 33.60
		ATOM	840	CB	SER .	A 1	L09	-6.166	53.759	60.437	1.00 41.44
	40	MOTA	841	OG	SER .	A 1	L09	-6.205	54.812	61.404	1.00 47.63
		MOTA	842	N	PRO .	A 1	110	-4.655	56.392	59.308	1.00 41.64
35		MOTA	843	CA	PRO .			-3.419	57.116	59.393	1.00 40.75
		MOTA	844	С	PRO .			~2.803	56.749	60.725	1.00 41.47
	AE	ATOM	845	0	PRO .			-1.676	57.080	61.009	1.00 42.30
	45	ATOM	846	CB	PRO .			-3.721	58.605	59.298	1.00 42.09
		ATOM	847	CG	PRO .			-5.224	58.719	59.132	1.00 48.77
		ATOM ATOM	848	CD	PRO .			-5.811	57.318	59.269	1.00 44.58
40		ATOM	849 850	N CA	LYS .			-3.578	56.017	61.518	1.00 36.35
	50	ATOM	851	C	LYS .			-3.167	55.535	62.819	1.00 36.74
	50	ATOM	852	õ	LYS			-2.669 -2.733	54.083 53.319	62.720	1.00 40.19
		ATOM	853	СВ	LYS			-4.341	55.606	63.678 63.807	1.00 40.53 1.00 41.91
		ATOM	854	CG	LYS			-4.362	56.838	64.708	1.00 41.91
		ATOM	855	CD	LYS			-5.421	57.854	64.309	1.00 71.21
45	55	ATOM	856	CE	LYS			-6.839	57.394	64.611	1.00100.00
45		ATOM	857	NZ	LYS			-7.853	58.120	63.819	1.00100.00
		ATOM	858	N	SER 2			-2.184	53.670	61.550	1.00 36.84
		MOTA	859	CA	SER			-1.714	52.296	61.358	1.00 34.35
		MOTA	860	C	SER 2			-0.518	51.917	62.225	1.00 35.57
	60	ATOM	861	0	SER .			0.533	52.548	62.166	1.00 32.49
		ATOM	862	СВ	SER A			-1.449	51.995	59.883	1.00 35.16
50		ATOM	863	OG	SER A	A 1	112	-0.682	50.814	59.762	1.00 31.94
		MOTA	864	N	SER A	A 1	113	-0.666	50.872	63.033	1.00 31.84
		MOTA	865	CA	SER Z	A 1	113	0.445	50.460	63.866	1.00 29.27

5		ATOM	866	С	SER A	113	1.601	49.927	63.040	1.00 33.37
-		ATOM	867	ō	SER A		2.715	49.792	63.497	1.00 32.95
		ATOM	868	СВ	SER A		0.052	49.498	64.945	1.00 29.45
		ATOM	869	ŌĞ	SER A		0.045	48.169	64.462	1.00 34.27
	5	ATOM	870	N	ALA A		1.357	49.628	61.797	1.00 33.69
	•	ATOM	871	CA	ALA A		2.437	49.134	60.981	1.00 34.05
		ATOM	872	c.	ALA A		3.239	50.287	60.388	1.00 37.83
10		ATOM	873	ō	ALA A		4.411	50.149	60.033	1.00 37.72
		ATOM	874	СВ	ALA A		1.845	48.292	59.852	1.00 34.51
	10	ATOM	875	N	LEU A		2.580	51.432	60.259	1.00 32.19
	••	ATOM	876	CA	LEU A		3.201	52.595	59.662	1.00 30.48
		ATOM	877	C	LEU A		3.509	53.745	60.565	1.00 35.32
		ATOM	878	ō	LEU A		2.902	54.012	61.604	1.00 35.25
		ATOM	879	CB	LEU A		2.358	53,156	58.507	1.00 30.53
15	15	ATOM	880	CG	LEU A		1,787	52.064	57.602	1.00 35.51
		ATOM	881		LEU A		0.812	52.710	56.637	1.00 35.12
		ATOM	882		LEU A		2.903	51.387	56.821	1.00 33.88
		ATOM	883	N	GLN A		4.490	54.457	60.096	1.00 34.00
		ATOM	884	CA	GLN A		4.926	55.656	60.737	1.00 32.52
	20	MOTA	885	С	GLN A		5.066	56.689	59.645	1.00 31.34
		ATOM	886	ō	GLN A		5.880	56.552	58.729	1.00 28.29
20		ATOM	887	CB	GLN A		6.232	55.540	61.496	1.00 32.66
		ATOM	888	CG	GLN A		6.419	56.813	62.322	1.00 41.25
		ATOM	889	CD	GLN A		7.777	56.897	62.952	1.00 50.08
	25	ATOM	890		GLN A		8.515	55.905	63.017	1.00 55.36
		MOTA	891		GLN A		8.090	58.081	63.438	1.00 38.23
		MOTA	892	N	TRP A		4.210	57.680	59.748	1.00 26.66
25		MOTA	893	CA	TRP A		4.148	58.785	58.827	1.00 26.04
23		MOTA	894	c	TRP A		4.912	59.978	59.375	1.00 34.56
	30	MOTA	895	ŏ	TRP A		4.467	60.589	60.364	1.00 36.83
		ATOM	896	СВ	TRP A		2.669	59.188	58.630	1.00 23.15
		ATOM	897	CG	TRP A		1.826	58.209	57.863	1.00 23.02
		ATOM	898		TRP A		1.052	57.224	58.397	1.00 26.39
		ATOM	899		TRP A		1.640	58.135	56.433	1.00 21.06
30	35	ATOM	900		TRP A		0.395	56.534	57.393	1.00 26.40
		ATOM	901		TRP A		0.735	57.087	56.184	1.00 27.99
		MOTA	902		TRP A		2.121	58.872	55.361	1.00 20.95
		ATOM	903		TRP A		0.352	56.753	54.886	1.00 28.21
		ATOM	904		TRP A		1.750	58.560	54.079	1.00 22.43
	40	ATOM	905		TRP A		0.872	57.512	53.847	1.00 24.28
		ATOM	906	N	LEU A		6.043	60.340	58.756	1.00 31.44
35		ATOM	907	CA	LEU A		6.745	61.506	59.276	1.00 36.67
		ATOM	908	С	LEU A		6.584	62.774	58.432	1.00 46.93
		ATOM	909	0	LEU A		6.434	62.705	57.210	1.00 51.17
	45	ATOM	910	СВ	LEU A		8.250	61.327	59.577	1.00 38.83
		ATOM	911	CG	LEU A		8.881	59.939	59.398	1.00 44.33
		ATOM	912		LEU A		10.392	60.065	59.569	1.00 42.12
40		ATOM	913		LEU A		8.351	58.950	60.426	1.00 49.99
40		ATOM	914	N	THR A		6.524	63.939	59.109	1.00 41.34
	50	ATOM	915	CA	THR A		6.449	65.260	58.468	1.00 38.89
		ATOM	916	C	THR A		7.847		58.034	1.00 40.14
		ATOM	917	ō	THR A		8.841	65.165	58.605	1.00 44.03
		ATOM	918	СВ	THR A		5.932	66.300	59.467	1.00 42.63
		ATOM	919		THR A		6.994	66.605	60.362	1.00 50.01
45	55	ATOM	920		THR A		4.769	65.668	60.224	1.00 36.78
45	-	ATOM	921	N	PRO A		7.963	66.440	57.020	1.00 33.41
		ATOM	922	CA	PRO A		9.275	66.781	56.517	1.00 33.18
		ATOM	923	c	PRO A		10.260	67.209	57.599	1.00 38.27
		ATOM	924	ŏ	PRO A		11.433	66.829	57.566	1.00 34.42
	60	ATOM	925	СВ	PRO A		9.068	67.840	55.416	1.00 33.54
		ATOM	926	ÇG	PRO A		7.582	67.823	55.097	1.00 34.86
50		ATOM	927	CD	PRO A		6.891	67.180	56.300	1.00 34.86
- -		ATOM	928	N	GLU A		9.751	67.982	58.563	1.00 38.03
		ATOM	929	CA	GLU A		10.534	68.474	59.681	1.00 41.03

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5		ATOM	930	C	GLU	Α	121	11.212	67.361	60.411	1.00 50.88
		ATOM	931	0	GLU	Α	121	12.279	67.548	60.977	1.00 54.97
		ATOM	932	CB	GLU	Α	121	9.742	69.325	60.699	1.00 43.28
		ATOM	933	CG	GLU	Α	121	8.220	69.071	60.702	1.00 64.72
	5	ATOM	934	CD	GLU	Α	121	7.398	70.118	59.988	1.00 86.07
		ATOM	935		GLU			7.007	71.131	60.538	1.00100.00
40		ATOM	936	OE2	GLU	А	121	7.108	69.803	58.739	1.00 59.72
10		ATOM	937	N	GLN	A	122	10.569	66.202	60.394	1.00 44.09
	4.0	ATOM	938	CA	GLN	Α	122	11.083	65.019	61.041	1.00 40.20
	10	ATOM	939	С	GLN			12.170	64.373	60.232	1.00 47.73
		ATOM	940	0	GLN			12.711	63.343	60.643	1.00 53.29
		ATOM	941	СВ	GLN			9.965	63.992	61.224	1.00 39.31
		ATOM	942	CG	GLN			9.057	64.441	62.361	1.00 30.23
15	1.5	ATOM	943	CD	GLN			7.756	63.691	62.438	1.00 38.25
.•	15	ATOM	944		GLN			6.899	63.804	61.548	1.00 53.34
		ATOM	945	NE2	GLN			7.592	62.938	63.521	1.00 18.98
		ATOM	946	N	THR			12.486	64.942	59.074	1.00 38.99
		ATOM	947	CA	THR			13.490	64.319	58.229	1.00 36.00
	20	ATOM	948	C	THR			14.755	65.034	58.264	1.00 35.30
	20	ATOM	949	0	THR			14.842	66.074	58.875	1.00 34.95
20		ATOM	950	CB	THR			13.067	64.145	56.759	1.00 38.25
		ATOM ATOM	951		THR			13.144	65.374	56.046	1.00 43.75
		ATOM	952 953					11.643	63.616	56.725	1.00 40.72
	25	ATOM	954	n Ca	SER SER			15.699 17.025	64.447	57.557	1.00 32.18
		ATOM	955	C.	SER			17.023	64.996 66.216	57.442	1.00 33.71
		ATOM	956	Ö	SER			17.537	67.268	56.553 56.883	1.00 39.04
25		ATOM	957	СВ	SER			18.023	63.992	56.859	1.00 37.73
25 .		ATOM	958	OG	SER			18.359	62.978	57.796	1.00 37.73
	30	ATOM	959	N	GLY			16.389	66.025	55.414	1.00 38.59
		ATOM	960	CA	GLY			16.280	67.034	54.396	1.00 39.90
		ATOM	961	C	GLY			15.290	68.094	54.749	1.00 46.83
		ATOM	962	0	GLY			15.347	69.171	54.172	1.00 49.78
		ATOM	963	N	LYS			14.391	67.788	55.678	1.00 41.09
30	35	ATOM	964	CA	LYS			13.396	68.761	56.126	1.00 41.26
		ATOM	965	С	LYS			12.498	69.307	55.020	1.00 47.42
		ATOM	966	0	LYS	Α	126	11.617	70.141	55.279	1.00 48.94
		ATOM	967	CB	LYS	Α	126	14.024	69.936	56.894	1.00 41.98
		ATOM	968	CG	LYS	Α	126	15.094	69.555	57.913	1.00 45.84
•	40	ATOM	969	CD	LYS	Α	126	14.535	68.838	59.135	1.00 58.74
25		ATOM	970	CE	LYS	Α	126	15.612	68.500	60.151	1.00 72.12
35		ATOM	971	NZ	LYS	Α	126	15.395	67.218	60.839	1.00 88.38
		ATOM	972	N	GLU	Α	127	12.722	68.858	53.792	1.00 41.82
	4.5	ATOM	973	CA	GLU			11.921	69.344	52.708	1.00 41.98
	45	ATOM	974	С	GLU			10.899	68.334	52.239	1.00 45.14
		ATOM	975	0	GLU			9.994	68.683	51.496	1.00 46.95
		ATOM	976	СВ	GLU			12.727	70.015	51.543	1.00 44.39
40		ATOM	977	CG	GLU			13.198	71.499	51.820	1.00 57.99
	50	MOTA	978	CD	GLU			12.331	72.659	51.301	1.00100.00
	30	MOTA	979		GLU			11.652	72.611	50.286	1.00100.00
		MOTA	980		GLU			12.387	73.758	52.054	1.00100.00
		ATOM	981	N	HIS			11.027	67.077	52.653	1.00 39.18
		MOTA	982	CA	HIS			10.068	66.072	52.210	1.00 39.43
	55	ATOM	983	C	HIS			9.636	65.148	53.316	1.00 42.09
45	رر	ATOM ATOM	984 985	O CB	HIS			10.366	64.955	54.281	1.00 45.34
		ATOM	986	CB CG	HIS HIS			10.628	65.194	51.097	1.00 42.16
		ATOM	987		HIS			10.947 9.943	65.936	49.854	1.00 47.24
		ATOM	988		HIS			12.159	66.423 66.262	49.029	1.00 49.12
	60	ATOM	989		HIS			10.559	67.031	49.322 48.026	1.00 51.13
	00	ATOM	990		HIS			11.888	66.953	48.026	1.00 49.97
50		ATOM	991	N	PRO			8.447	64.572	53.171	1.00 50.87 1.00 32.55
		ATOM	992	CA	PRO			7.968	63.650	54.163	1.00 32.35
		ATOM	993	C			129	8.636	62.328	53.900	1.00 34.90
				-				0.000	32.320	30.300	55 54.50

5		MOTA	994	0	PRO A	A 129	9.481	62.214	53.021	1.00 35.46
		MOTA	995	CB	PRO 2	A 129	6.466	63.490	53.986	1.00 31.94
		MOTA	996	CG	PRO 2	A 129	6.133	64.104	52.649	1.00 36.83
	_	MOTA	997	CD	PRO 2	A 129	7.384	64.850	52.185	1.00 32.71
	5	ATOM	998	N	TYR A	A 130	8.248	61.342	54.659	1.00 29.47
		MOTA	999	CA	TYR A	A 130	8.826	60.025	54.548	1.00 29.35
		ATOM	1000	С	TYR A	A 130	7.856	59.046	55.156	1.00 31.83
10		ATOM	1001	0	TYR A	A 130	7.138	59.375	56.093	1.00 29.84
	4.0	ATOM	1002	CB	TYR 2	A 130	10.098	60.029	55.433	1.00 30.54
	10	MOTA	1003	CG		A 130	11.083	58.886	55.285	1.00 29.76
		MOTA	1004		TYR A		10.845	57.630	55.845	1.00 26.16
		ATOM	1005		TYR A		12.290	59.110	54.619	1.00 30.28
		MOTA	1006		TYR 2		11.795	56.621	55.721	1.00 17.87
15	16	ATOM	1007	CE2			13.253	58.114	54.479	1.00 27.75
, 0	15	ATOM	1008	CZ		A 130	12.983	56.866	55.031	1.00 25.76
		ATOM	1009	OH		A 130	13.899	55.864	54.894	1.00 40.52
		MOTA	1010	N		A 131	7.832	57.842	54.647	1.00 31.12
		MOTA	1011	CA		A 131	6.994	56.868	55.303	1.00 30.43
	20	ATOM	1012	C		A 131	7.691	55.568	55.289	1.00 33.91
	20	ATOM	1013	0		A 131	8.398	55.257	54.397	1.00 33.68
20		MOTA	1014	CB		A 131	5.679	56.761	54.530	1.00 26.16
		MOTA	1015 1016	CG		A 131	5.065	55.367	54.600	1.00 21.68
		ATOM	1017		LEU A		4.163	55.206	55.797	1.00 17.56
	25	ATOM ATOM	1017	N	LEU A	A 132	4.222 7.533	55.008	53.380	1.00 13.86
	43	ATOM	1019	CA		A 132	8.129	54.828	56.348	1.00 29.24 1.00 33.44
		ATOM	1020	C		A 132	7.299	53.527 52.519	56.323 57.157	1.00 33.44
25		ATOM	1021	õ		A 132	6.344	52.889	57.837	1.00 41.08
25		ATOM	1022	СВ		A 132	9.621	53.670	56.791	1.00 36.40
	30	ATOM	1023	CG		A 132	9.763	53.895	58.256	1.00 38.11
		ATOM	1024		PHE A		9.601	52.821	59.053	1.00 37.18
		ATOM	1025		PHE A		10.123	55.158	58.803	1.00 43.89
		ATOM	1026		PHE A		9.771	52.936	60.422	1.00 41.04
		MOTA	1027	CE2	PHE A	A 132	10.289	55.258	60.174	1.00 47.72
30	35	ATOM	1028	CZ	PHE A	A 132	10.131	54.143	60.986	1.00 44.34
		ATOM	1029	N		A 133	7.612	51.221	57.002	1.00 33.47
		ATOM	1030	CA	SER A	A 133	6.744	50.228	57.629	1.00 29.86
		MOTA	1031	С	SER A	A 133	7.499	49.221	58.504	1.00 31.53
		ATOM	1032	0	SER A	A 133	8.724	49.146	58.531	1.00 33.16
	40	MOTA	1033	CB	SER A	A 133	5.942	49.481	56.535	1.00 33.19
25		ATOM	1034	OG	SER A	A 133	6.757	48.480	55.926	1.00 50.66
35		MOTA	1035	N	GLN A	A 134	6.703	48.466	59.294	1.00 24.61
		ATOM	1036	CA		A 134	7.283	47.422	60.134	1.00 22.55
	4.5	ATOM	1037	С		A 134	6.268	46.321	60.398	1.00 27.28
	45	ATOM	1038	0		A 134	5.161	46.566	60.809	1.00 25.09
		MOTA	1039	CB		A 134	7.711	48.041	61.464	1.00 23.29
		ATOM	1040	CG		A 134	8.218	46.987	62.454	1.00 25.96
40		ATOM	1041	CD		A 134	9.423	46.290	61.872	1.00 25.65
	50	MOTA	1042		GLN A		10.296	46.876	61.263	1.00 26.36
	50	MOTA MOTA	1043		GLN A		9.445	44.965	62.095	1.00 21.75
			1044 1045	N		A 135	6.435	45.124	59.820	1.00 29.60
		ATOM ATOM	1045	CA C		A 135	5.291	44.220	59.755	1.00 32.30
		ATOM	1047	0		A 135 A 135	5.442 4.597	43.006	60.662	1.00 39.58
4.0	55	ATOM	1047	CB		A 135	5.098	42.144	60.739 58.320	1.00 40.94
45	7,5	ATOM	1049	SG		A 135	3.976	43.794 44.922	57.445	1.00 35.40
		ATOM	1050	N		A 136	6.582	42.949		1.00 41.22
		ATOM	1051	CA		A 136	6.715	41.982	61.345 62.417	1.00 37.37 1.00 35.71
		ATOM	1052	C		A 136	6.589	42.645	63.797	1.00 33.71
	60	ATOM	1053	ŏ		A 136	6.878	43.803	63.797	1.00 31.90
		ATOM	1054	ČВ		A 136	8.077	41.311	62.295	1.00 30.34
50		ATOM	1055	CG		A 136	8.076	39.878	62.847	1.00 37.24
		ATOM	1056	CD		A 136	9.483	39.511	63.235	1.00 36.48
		ATOM	1057		GLN A		10.366	40.328	63.356	1.00 24.49

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5		ATOM	1058		GLN			9.665	38.201	63.443	1.00 22.19
		ATOM	1059	N	ALA			5.850	41.899	64.648	1.00 28.56
		ATOM ATOM	1060	CA C	ALA			5.235	40.581	64.351	1.00 28.89
	5	ATOM	1061 1062	ò	ALA			3.860 3.679	40.503 39.688	63.630	1.00 31.83
	-	ATOM	1063	СВ	ALA			5.091	39.742	62.738 65.625	1.00 29.67
		ATOM	1064	N	ILE			2.863	41.285	64.070	1.00 28.91 1.00 27.07
10		ATOM	1065	CA	ILE			1.553	41.176	63.445	1.00 23.90
		MOTA	1066	С	ILE			0.960	42.492	63.053	1.00 28.69
	10	MOTA	1067	0	ILE			-0.144	42.822	63.426	1.00 31.92
		ATOM	1068	CB	ILE	А	138	0.641	40.357	64.339	1.00 25.41
		MOTA	1069	CG1	ILE	Α	138	0.871	40.811	65.801	1.00 27.32
		MOTA	1070		ILE			1.162	38.938	64.191	1.00 16.34
15	1.5	MOTA	1071		ILE			-0.275	40.615	66.826	1.00 20.22
70	15	MOTA	1072	N	HIS			1.718	43.223	62.265	1.00 24.05
		ATOM	1073	CA	HIS			1.322	44.511	61.824	1.00 24.05
		ATOM	1074	C	HIS			0.982	44.579	60.351	1.00 34.40
		ATOM	1075 1076	O CB	HIS			0.539	45.625	59.888	1.00 35.89
	20	ATOM ATOM	1077	CG	HIS			2.439 2.689	45.519	62.173	1.00 24.63
	20	ATOM	1078		HIS			1.679	45.619 45.970	63.657 64.571	1.00 27.97
20		ATOM	1079		HIS			3.835	45.437	64.356	1.00 27.75
		ATOM	1080		HIS			2.222	45.983	65.770	1.00 26.19
		ATOM	1081		HIS			3.517	45.668	65.671	1.00 27.42
	25	ATOM	1082	N	CYS			1.181	43.490	59.598	1.00 30.28
		ATOM	1083	CA	CYS			0.832	43.517	58.181	1.00 28.08
		MOTA	1084	С	CYS	Α	140	-0.671	43.765	58.011	1.00 28.98
25		MOTA	1085	0	CYS	Α	140	-1.111	44.449	57.066	1.00 30,00
	20	ATOM	1086	CB	CYS			1.181	42.213	57.447	1.00 28.82
	30	ATOM	1087	SG	CYS			1.330	42.483	55.661	1.00 34.37
		ATOM	1088	N	ARG			-1.440	43.168	58.949	1.00 20.78
		ATOM	1089	CA	ARG			-2.884	43.252	58.996	1.00 20.33
		ATOM	1090	C	ARG			-3.286	44.684	59.003	1.00 32.37
30	35	ATOM ATOM	1091 1092	O CB	ARG			-4.355	45.032	58.510	1.00 35.81
30	33	ATOM	1092	CG	ARG ARG			-3.557 -3.081	42.498 42.891	60.156	1.00 14.60
		ATOM	1094	CD	ARG			-3.576	41.978	61.568 62.715	1.00 20.94 1.00 19.99
		ATOM	1095	NE	ARG			-2.911	40.690	62.786	1.00 19.99
		ATOM	1096	CZ	ARG			-3.140	39.707	63.648	1.00 18.77
	40	ATOM	1097		ARG			-4.029	39.739	64.634	1.00 20.76
		ATOM	1098		ARG			-2.415	38.640	63.508	1.00 24.20
35		MOTA	1099	N	ALA	Α	142	-2.408	45.511	59.580	1.00 28.35
		MOTA	1100	CA	ALA	Α	142	-2.668	46.940	59.657	1.00 27.60
	46	ATOM	1101	С	ALA			-2.369	47.652	58.345	1.00 34.33
	45	ATOM	1102	0	ALA			-2.620	48.835	58.203	1.00 34.36
		ATOM	1103	СВ	ALA			-1.994	47.616	60.843	1.00 27.67
		ATOM ATOM	1104 1105	N CA	ILE			-1.824	46.922	57.382	1.00 32.39
40		ATOM	1105	c	ILE			-1.537 -2.520	47.499 46.994	56.099 55.067	1.00 30.38 1.00 37.79
	50	ATOM	1107	Ö	ILE			-2.885	47.709	54.152	1.00 37.79
		ATOM	1108	СB	ILE			-0.142	47.228	55.613	1.00 32.06
		ATOM	1109		ILE			0.827	48.062	56.414	1.00 32.00
		ATOM	1110		ILE			-0.074	47.654	54.143	1.00 34.02
		ATOM	1111		ILE			2.258	47.774	55.988	1.00 42.10
45	55	MOTA	1112	N	LEU	Α	144	-2.939	45.749	55.218	1.00 32.50
-		MOTA	1113	CA	LEU			-3.873	45.142	54.291	1.00 32.36
		ATOM	1114	С	LEU			-4.435	43.838	54.849	1.00 40.36
		ATOM	1115	0	LEU			-3.959	43.278	55.852	1.00 33.27
	40	ATOM	1116	CB	LEU			-3.250	44.936	52.894	1.00 31.58
	60	ATOM	1117	CG	LEU			-1.923	44.170	52.917	1.00 33.31
50		ATOM	1118		LEU			-2.147	42.770	52.352	1.00 32.07
50		ATOM	1119		LEU			-0.836	44.897	52.110	1.00 28.67
		ATOM ATOM	1120	N CA	PRO			-5.490 -6.090	43.347	54.213	1.00 40.02
		ALON	1121	CA	PRO	м	143	-6.080	42.129	54.715	1.00 37.86

5		ATOM	1122	С	PRO A	A 145	-5.264	40.941	54.286	1.00 37.87
		ATOM	1123	0	PRO A		-4.819	40.831	53.144	1.00 35.27
		ATOM	1124	СВ	PRO A		-7.530	42.080	54.220	1.00 38.81
		ATOM	1125	CG	PRO A		-7.778	43.393	53.492	1.00 41.34
	5	ATOM	1126	CD	PRO A	A 145	-6.432	44.093	53.341	1.00 36.69
		ATOM	1127	N	CYS 7	A 146	-5.041	40.056	55.233	1.00 36.18
		MOTA	1128	CA	CYS A	A 146	-4.250	38.882	54.958	1.00 35.60
10		MOTA	1129	С	CYS A	A 146	-4.358	37.859	56.069	1.00 33.04
		ATOM	1130	0	CYS A	A 146	-5.067	38.062	57.050	1.00 30.78
	10	MOTA	1131	CB		A 146	-2.761	39.287	54.813	1.00 36.08
		ATOM	1132	SG		A 146	-2.087	40.108	56.302	1.00 39.43
		ATOM	1133	N		A 147	-3.637	36.755	55.883	1.00 29.33
		ATOM	1134	CA		A 147	-3.517	35.703	56.875	1.00 29.71
15	1.5	ATOM	1135	C		A 147	-2.254	36.131	57.628	1.00 38.75
,,	15	MOTA	1136	0		A 147	-1.141	35.926	57.135	1.00 40.79
		ATOM	1137	СВ		A 147	-3.322	34.352	56.206	1.00 28.99
		ATOM	1138	CG		A 147	-4.672	33.707	55.894	1.00 25.73
		ATOM	1139	CD		A 147	-4.562	32.532	54.960	1.00 39.92
	20	ATOM	1140		GLN A		-4.217	32.668	53.775	1.00 43.89
	20	ATOM	1141		GLN A		-4.828	31.368	55.499	1.00 26.36
20		ATOM	1142	N		A 148	-2.425	36.834	58.765 59.474	1.00 32.68
		MOTA	1143	CA	ASP A		-1.287	37.362		1.00 33.50
		ATOM ATOM	1144 1145	0		A 148 A 148	-0.629 -0.622	36.377 36.563	60.371 61.584	1.00 33.13 1.00 31.30
	25	ATOM	1145	СВ		A 148	-1.633	38.642	60.253	1.00 31.30
	23	ATOM	1147	CG		A 148	-0.535	39.666	60.332	1.00 37.78
		ATOM	1148		ASP A		0.564	39.540	59.836	1.00 47.89
25		ATOM	1149		ASP A		-0.913	40.737	60.952	1.00 48.63
25		ATOM	1150	N		A 149	-0.080	35.345	59.742	1.00 29.15
	30	ATOM	1151	CA		A 149	0.584	34.251	60.422	1.00 28.25
		ATOM	1152	c		A 149	1.805	33.831	59.625	1.00 34.92
		ATOM	1153	ō		A 149	1.757	33.764	58.410	1.00 34.47
		ATOM	1154	СВ		A 149	-0.403	33.087	60.674	1.00 24.79
		ATOM	1155		THR A		0.241	32.059	61.352	1.00 37.15
30	35	MOTA	1156		THR A		-0.905	32.527	59.345	1.00 26.56
		ATOM	1157	N	PRO A	A 150	2.910	33.575	60.323	1.00 34.69
		MOTA	1158	CA	PRO 2	A 150	4.142	33.217	59.659	1.00 31.06
		MOTA	1159	С	PRO A	A 150	4.087	31.813	59.131	1.00 36.66
		MOTA	1160	0	PRO 2	A 150	4.995	31.356	58.450	1.00 36.37
	40	ATOM	1161	CB	PRO 2	A 150	5.245	33.327	60.712	1.00 31.18
25		ATOM	1162	CG	PRO 2	A 150	4.570	33.471	62.077	1.00 36.95
35		MOTA	1163	CD	PRO 2	A 150	3.078	33.589	61.823	1.00 34.62
		MOTA	1164	N	SER	A 151	2.992	31.150	59.452	1.00 31.62
		MOTA	1165	CA		A 151	2.778	29.791	59.029	1.00 27.35
	45	ATOM	1166	С		A 151	2.357	29.738	57.564	1.00 32.97
		MOTA	1167	0		A 151	2.344	28.703	56.928	1.00 34.25
		MOTA	1168	CB		A 151	1.714	29.203	59.905	1.00 25.95
40		MOTA	1169	0G		A 151	0.483	29.685	59.439	1.00 49.35
	50	ATOM	1170	N		A 152	1.997	30.887	57.024	1.00 34.36
	J U	ATOM	1171	CA		A 152	1.595	31.015	55.623	1.00 33.74
		MOTA	1172	C		A 152	2.705	31.764	54.847	1.00 37.45
		ATOM	1173	0		A 152	3.295	32.761	55.313	1.00 37.63
		MOTA	1174	CB CC1		A 152	0.203	31.697	55.427	1.00 32.61
45	55	ATOM	1175 1176			A 152	-0.184	31.767	53.963	1.00 31.50
45	22	ATOM				A 152	-0.915	30.975	56.149	1.00 31.29
		ATOM	1177 1178	N		A 153	2.999	31.289	53.654	1.00 26.98
		MOTA MOTA	1178	CA		A 153 A 153	4.002 3.469	31.927 32.141	52.866	1.00 25.81 1.00 33.94
		ATOM	1179	С 0		A 153	2.826	31.251	51.473 50.936	1.00 33.94
	60	ATOM	1181	СВ		A 153	5.252	31.231	52.841	1.00 32.91
	00	MOTA	1182	CG		A 153	6.383	31.760	53.583	1.00 24.70
50		ATOM	1183	CD		A 153	7.641	30.893	53.616	1.00 34.00
		ATOM	1184	CE		A 153	8.121	30.506	55.015	1.00 39.37
		ATOM	1185	NZ		A 153	9.556	30.152	55.112	1.00 26.03
			1100		~		5.550	30.132	55.112	7.00 50.03

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5		ATOM	1186		LEU A		3.732	33.321	50.896	1.00 32.13
		ATOM	1187	CA	LEU A		3.285	33.639	49.544	1.00 30.67
		MOTA	1188	С	LEU A		4.279	34.475	48.789	1.00 40.67
	_	MOTA	1189	0	LEU A		5.264	35.000	49.344	1.00 42.56
	5	ATOM	1190	СВ	LEU A		1.966	34.432	49.515	1.00 30.10
		MOTA	1191	CG	LEU A		2.084	35.793	50.207	1.00 35.20
10		MOTA	1192	CD1	LEU A	154	0.989	36.716	49.690	1.00 37.21
10		ATOM	1193	CD2	LEU A	154	1.934	35.608	51.715	1.00 33.07
		ATOM	1194	N	THR A	. 155	3.963	34.610	47.499	1.00 37.82
	10	MOTA	1195	CA	THR A	155	4.728	35.449	46.596	1.00 38.44
		ATOM	1196	С	THR A	155	3.934	36.730	46.389	1.00 41.52
		ATOM	1197	0	THR A	155	2.738	36.775	46.674	1.00 43.95
		ATOM	1198	CB	THR A	155	5.041	34.814	45.230	1.00 36.99
15		ATOM	1199	OG1	THR A	155	3.886	34.201	44.584	1.00 32.59
10	15	ATOM	1200	CG2	THR A	155	6.133	33.790	45.404	1.00 18.24
		ATOM	1201	N	TYR A	156	4.563	37.768	45.892	1.00 33.87
		ATOM	1202	CA	TYR A	156	3.835	39.003	45.683	1.00 32.49
		ATOM	1203	С	TYR A	156	4.509	39.922	44.717	1.00 37.91
		ATOM	1204	0	TYR A		5.725	39.940	44.562	1.00 39.04
	20	ATOM	1205	CB	TYR A		3.534	39.795	46.983	1.00 31.16
20		ATOM	1206	CG	TYR A		4.642	40.731	47.471	1.00 28.94
20		ATOM	1207	CD1	TYR A		4.817	42.021	46.969	1.00 30.33
		ATOM	1208		TYR A		5.525	40.303	48.465	1.00 30.43
		ATOM	1209		TYR A		5.829	42.853	47.459	1.00 36.89
	25	ATOM	1210		TYR A		6.553	41.104	48.960	1.00 31.47
	23	ATOM	1211	CZ	TYR A		6.690	42.396	48.462	1.00 43.34
		ATOM	1212	OH	TYR A		7.701	43.180	48.956	1.00 36.86
25		ATOM					3.657	40.689		1.00 36.35
25			1213	N	THR A				44.101	
	30	ATOM	1214	CA	THR A		4.036	41.691	43.171	1.00 38.49
	30	ATOM	1215	C	THR A		3.346	42.942	43.611	1.00 42.61
		ATOM	1216	0	THR A		2.228	42.913	44.143	1.00 38.45
		ATOM	1217	CB	THR A		3.631	41.316	41.751	1.00 39.73
		ATOM	1218		THR A		2.380	40.655	41.803	1.00 55.71
30	25	ATOM	1219		THR A		4.680	40.370	41.212	1.00 26.71
30	35	ATOM	1220	N	ALA A		4.037	44.025	43.404	1.00 41.36
		ATOM	1221	CA	ALA A		3.488	45.273	43.789	1.00 41.08
		ATOM	1222	C ,	ALA A		3.869	46.401	42.839	1.00 50.77
		ATOM	1223	0	ALA A		4.919	46.390	42.179	1.00 53.47
	40	ATOM	1224	CB	ALA A		3.910	45.570	45.212	1.00 39.87
	40	ATOM	1225	N	GLU A		2.974	47.376	42.788	1.00 43.90
35		MOTA	1226	CA	GLU A		3.107	48.604	42.023	1.00 42.27
55		ATOM	1227	C	GLU A		2.451	49.705	42.843	1.00 42.17
		ATOM	1228	0	GLU A		1.257	49.630	43.227	1.00 41.00
	4.5	ATOM	1229	СВ	GLU A		2.641	48.521	40.571	1.00 43.72
	45	ATOM	1230	CG	GLU A		1.943	47.197	40.255	1.00 62.90
		ATOM	1231	CD	GLU A		1.502	47.156	38.835	1.00 91.28
		ATOM	1232	OE1	GLU A	159	2.202	46.696	37.955	1.00 77.84
40		ATOM	1233	OE2	GLU A	159	0.322	47.707	38.644	1.00100.00
		ATOM	1234	N	VAL A	160	3.263	50.686	43.197	1.00 34.67
	50	ATOM	1235	CA	VAL A	160	2.738	51.717	44.044	1.00 36.57
		ATOM	1236	C	VAL A	160	3.024	53.091	43.533	1.00 43.02
		ATOM	1237	0	VAL A	160	4.121	53.380	43.050	1.00 42.71
		ATOM	1238	CB	VAL A	160	3.180	51.530	45.500	1.00 40.73
		ATOM	1239	CG1	VAL A	160	3.988	50.239	45.644	1.00 38.56
45	55	ATOM	1240	CG2	VAL A	160	4.006	52.728	45.963	1.00 40.46
		ATOM	1241	N	SER A	161	2.002	53.922	43.653	1.00 41.79
		ATOM	1242	CA	SER A	161	2.076	55.292	43.185	1.00 42.07
		ATOM	1243	C	SER A		2.532	56.204	44.270	1.00 44.28
		ATOM	1244	ō	SER A		2.047	56.121	45.403	1.00 43.60
	60	ATOM	1245	СВ	SER A		0.751	55.801	42.635	1.00 43.32
		ATOM	1246	OG	SER A		0.971	56.850	41.726	1.00 49.40
50 .		ATOM	1247	N	VAL A		3.447	57.080	43.896	1.00 36.49
		ATOM	1248	CA	VAL		3.979	58.019	44.838	1.00 30.49
		ATOM	1249	C	VAL A		4.273	59.319	44.148	1.00 34.99
		ATOR	1613	v	ALTH 1	. 102	7.2/3	09.319	33.130	2.00 72.37

5		ATOM	1250	0	VAL A	A 162	4.470	59.354	42.932	1.00 44.41
		ATOM	1251	СВ		A 162	5.300	57.498	45.402	1.00 35.97
		ATOM	1252		VAL A		5.084	56.219	46.188	1.00 36.12
		ATOM	1253		VAL		6.222	57.194	44.239	1.00 35.42
	5	ATOM	1254	N		A 163	4.332	60.377	44.942	1.00 32.95
	3	ATOM	1255	CA		A 163	4.664	61.662	44.400	1.00 31.07
		ATOM	1256	C		A 163	5.966	61.496	43.652	1.00 39.67
10		ATOM	1257	õ		A 163	6.919	60.892	44.142	1.00 42.78
	10	ATOM	1258	CB		A 163	4.780	62.562	45.618	1.00 31.62
	10	ATOM	1259	CG		A 163	3.946	61.893	46.714	1.00 33.93
		ATOM	1260	CD		A 163	3.652	60.480	46.259	1.00 28.53
		ATOM	1261	N		A 164	5.962	61.978	42.436	1.00 38.52
		ATOM	1262	CA		A 164	7.086	61.860	41.539	1.00 39.97
15	1.5	ATOM	1263	C		A 164	8.451	62.222	42.088	1.00 42.75
, -	15	ATOM	1264	0		A 164	9.453	61.708	41.593	1.00 44.47
		ATOM	1265	CB		A 164	6.828	62.479	40.177	1.00 44.67
		ATOM	1266	CG		A 164	6.004	63.758	40.257	1.00 78.05
		MOTA	1267	CD		A 164	6.651	64.918	39.497	1.00100.00
		MOTA	1268	CE		A 164	6.016	66.289	39.772	1.00100.00
	20	ATOM	1269	NZ	LYS .	A 164	6.679	67.075	40.835	1.00100.00
20		ATOM	1270	N	GLU .	A 165	8.519	63.097	43.082	1.00 37.25
		ATOM	1271	CA	GLU .	A 165	9.814	63.489	43.665	1.00 39.56
		ATOM	1272	С	GLU .	A 165	10.333	62.462	44.677	1.00 46.39
		MOTA	1273	0	GLU .	A 165	11.531	62.318	44.927	1.00 48.93
	25	ATOM	1274	CB	GLU .	A 165	9.797	64.902	44.297	1.00 42.10
		ATOM	1275	CG	GLU .	A 165	8.602	65.156	45.257	1.00 58.16
		ATOM	1276	CD		A 165	7.214	64.970	44.664	1.00 88.01
25		ATOM	1277			A 165	6.994	64.757	43.475	1.00 79.46
		ATOM	1278			A 165	6.266	65.050	45.575	1.00 70.27
	30	ATOM	1279	N		A 166	9.398	61.733	45.265	1.00 40.39
		ATOM	1280	CA		A 166	9.696	60.733	46.254	1.00 36.56
		ATOM	1281	С		A 166	9.934	59.377	45.640	1.00 47.57
		ATOM	1282	Ō		A 166	9.366	59.080	44.581	1.00 52.86
		ATOM	1283	СВ		A 166	8.525	60.630	47.250	1.00 31.92
30	35	ATOM	1284	CG		A 166	8.315	61.912	48.057	1.00 29.18
	-	ATOM	1285			A 166	7.363	61.590	49.189	1.00 25.96
		ATOM	1286			A 166	9.635	62.467	48.622	1.00 23.78
		ATOM	1287	N		A 167	10.769	58.564	46.328	1.00 34.75
		ATOM	1288	CA		A 167	11.077	57.218	45.908	1.00 30.00
	40	ATOM	1289	c.		A 167	10.332	56.229	46.771	1.00 38.80
	70	ATOM	1290	ŏ		A 167	9.902	56.532	47.879	1.00 40.91
35		ATOM	1291	СВ		A 167	12.549	56.860	46.048	1.00 31.28
		ATOM	1292			A 167	12.854	55.542	45.329	1.00 28.20
		ATOM	1293			A 167	13.456	57.964	45.565	1.00 20.20
	45	ATOM	1294	N			10.217	55.019	46.257	
	45					A 168		53.019		1.00 36.46
		ATOM	1295	CA		A 168	9.584		46.979	1.00 35.14
		ATOM	1296	С		A 168	10.418	52.662	46.836	1.00 43.27
40		ATOM	1297	0		A 168	10.889	52.343	45.733	1.00 44.74
	50	ATOM	1298	CB		A 168	8.149	53.700	46.550	1.00 34.20
	50	ATOM	1299	N		A 169	10.603	51.960	47.975	1.00 35.27
		ATOM	1300	CA		A 169	11.323	50.696	48.069	1.00 29.39
		ATOM	1301	С		A 169	10.491	49.635	48.797	1.00 33.87
		ATOM	1302	0		A 169	9.604	49.918	49.613	1.00 31.21
		ATOM	1303	CB		A 169	12.721	50.835	48.656	1.00 28.62
45	55	ATOM	1304	CG		A 169	13.593	51.810	47.891	1.00 35.90
		ATOM	1305			A 169	14.953	51.819	48.558	1.00 39.38
		ATOM	1306	CD2	LEU	A 169	13.765	51.394	46.432	1.00 37.35
		ATOM	1307	N		A 170	10.758	48.381	48.479	1.00 34.23
		ATOM	1308	CA	MET	A 170	10.012	47.291	49.069	1.00 31.07
	60	ATOM	1309	С		A 170	10.874	46.083	49.287	1.00 34.13
		ATOM	1310	0		A 170	11.995	45.973	48.775	1.00 35.20
50		ATOM	1311	СВ		A 170	8.842	46.882	48.154	1.00 31.95
		ATOM	1312	CG		A 170	7.751	47.934	48.116	1.00 33.13
		ATOM	1313	SD		A 170	6.105	47.253	47.815	1.00 34.54

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•		ATOM	1314	CE	MET A		5.820	46.349	49.363	1.00 32.25
		ATOM	1315	N	SER A		10.332	45.165	50.057	1.00 28.20
		ATOM	1316 1317	CA	SER A		11.064 10.929	43.953 43.054	50.297	1.00 28.47
	5	ATOM	1317	0	SER A		10.329	43.054	49.049	1.00 32.01
	,	ATOM ATOM	1319	СВ	SER A		10.662	43.265	49.089	1.00 30.93
		ATOM	1320	OG	SER A		9,297	42.920	51.606	
10		ATOM	1321	N	ALA A		11.401	43.543	51.581 47.912	1.00 32.90 1.00 28.84
		ATOM	1322	CA	ALA A		11.286	42.773	46.691	1.00 28.84
	10	ATOM	1323	C	ALA A		12.241	43.258	45.644	1.00 23.40
	10	ATOM	1324	õ	ALA A		13.060	44.147	45.881	1.00 37.03
		ATOM	1325	СВ	ALA A		9.884	42.969	46.120	1.00 29.48
		ATOM	1326	N	ILE A		12.104	42.686	44.452	1.00 39.49
46		ATOM	1327	ĊA	ILE A		12.966	43.120	43.382	1.00 38.64
15	15	ATOM	1328	C	ILE A		12.418	44.343	42.648	1.00 44.83
		ATOM	1329	0	ILE A		11.269	44.394	42.193	1.00 40.97
		ATOM	1330	СВ	ILE A		13.549	42.027	42.479	1.00 38.79
		ATOM	1331		ILE A		14.258	40.970	43.302	1.00 37.40
		ATOM	1332		ILE A		14.606	42.621	41.570	1.00 38.88
	20	ATOM	1333		ILE A		15.770	41.069	43.193	1.00 25.93
20		MOTA	1334	N	ARG A	174	13.286	45.345	42.584	1.00 43.21
_•		ATOM	1335	CA	ARG A	174	12.997	46.567	41.917	1.00 42.34
		ATOM	1336	С	ARG A	174	12.630	46.173	40.516	1.00 47.54
		MOTA	1337	0	ARG A	174	13.478	45.667	39.770	1.00 42.08
	25	ATOM	1338	CB	ARG A	174	14.254	47.422	41.937	1.00 42.47
		ATOM	1339	CG	ARG A	174	14.231	48.450	43.075	1.00 53.40
		ATOM	1340	CD	ARG A	174	15.617	48.917	43.515	1.00 33.80
25		ATOM	1341	NE	ARG A	174	16.036	50.083	42.756	1.00 53.32
		ATOM	1342	CZ	ARG A		17.221	50.208	42.181	1.00 97.11
	30	ATOM	1343		ARG A		18.132	49.243	42.266	1.00100.00
		ATOM	1344		ARG A		17.503	51.321	41.489	1.00100.00
		ATOM	1345	N	ASP A		11.356	46.356	40.195	1.00 51.12
		ATOM	1346	CA	ASP A		10.858	45.981	38.882	1.00 53.89
30	25	ATOM	1347	C	ASP A		10.778	47.128	37.885	1.00 58.32
30	35	ATOM	1348	0	ASP A		10.455	46.901	36.727	1.00 56.00
		ATOM	1349	СВ	ASP A		9.533	45.186	38.948	1.00 57.16
		ATOM	1350	CG .			9.196	44.446	37.675	1.00 81.25
		MOTA	1351		ASP A		10.034	44.118	36.851	1.00 83.53
	40	ATOM ATOM	1352 1353	N	ASP A GLY A		7.910 11.062	44.176 48.356	37.558 38.331	1.00 92.45
	40	ATOM	1354	CA	GLY A		11.002	49.498	37.438	1.00 58.24 1.00 57.71
35		MOTA	1355	C	GLY A		9.969	50.546	37.773	1.00 58.98
		ATOM	1356	Ö	GLY A		9.090	50.371	38.620	1.00 52.04
		ATOM	1357	N	GLU A		10.110	51.649	37.050	1.00 63.72
	45	ATOM	1358	CA	GLU A		9.267	52.812	37.172	1.00 67.79
		ATOM	1359	C	GLU A		8.874	53.388	35.817	1.00 86.22
		ATOM	1360	0	GLU A		9.614	53.364	34.830	1.00 91.14
40		ATOM	1361	CB	GLU A		9.986	53.902	38.006	1.00 68.25
40		MOTA	1362	CG	GLU A		11.432	54.145	37.519	1.00 71.58
	50	MOTA	1363	CD	GLU A	177	12.183	55.088	38.404	1.00 85.08
		MOTA	1364	OE1	GLU A	177	13.045	54.733	39.198	1.00100.00
		MOTA	1365	OE2	GLU A	177	11.765	56.316	38.264	1.00 56.71
		MOTA	1366	N	THR A	178	7.671	53.924	35.835	1.00 84.76
		MOTA	1367	CA	THR A	178	6.684	54.686	35.042	1.00 84.81
45	55	MOTA	1368	С	THR A	178	6.024	55.810	35.855	1.00 90.37
		MOTA	1369	0	THR A	178	5.664	55.655	36.996	1.00 91.10
		MOTA	1370	CB	THR A		5.618	53.713	34.561	1.00 89.82
		ATOM	1371	OG1			5.283	52.830	35.636	1.00 80.25
	CO	MOTA	1372		THR A		6.161	52.898	33.396	1.00 93.46
	60	MOTA	1373	N	PRO A		5.921	56.984	35.217	1.00 87.05
E0		ATOM	1374	CA	PRO A		5.365	58.187	35.845	1.00 86.61
50		ATOM	1375	C	PRO A		3.857	58.419	35.531	1.00 89.04
		ATOM	1376	0	PRO A		3.444	59.516	35.140	1.00 91.15
	•	MOTA	1377	CB	PRO A	179	6.176	59.345	35.301	1.00 88.63

5		3.0004	1378	cc	nno	. 170	C (53	FO 047	22 225	
3		atom atom	1379	CG		A 179 A 179	6.657 6.426	58.947 57.345	33.895	1.00 92.62
		ATOM	1380	N		A 180	3.020	57.345	33.902 35.694	1.00 87.63 1.00 82.31
		ATOM	1381	CA		A 180	1.616	57.568	35.310	1.00 82.31
	5	ATOM	1382	c		A 180	0.629	56.743	36.166	1.00 90.72
	-	ATOM	1383	0		A 180	0.533	55.519	36.072	1.00 91.13
		ATOM	1384	CB		A 180	1.458	57.196	33.827	1.00 82.12
10		ATOM	1385	CG		A 180	0.087	57.651	33.327	1.00 95.94
		MOTA	1386	OD1	ASP .	A 180	-0.155	58.858	33.337	1.00100.00
	10	ATOM	1387	OD2	ASP .	A 180	-0.714	56.801	32.946	1.00 94.36
		ATOM	1388	N	PRO .	A 181	-0.060	57.456	37.086	1.00 92.45
		ATOM	1389	CA		A 181	-1.212	56.934	37.795	1.00 92.02
		ATOM	1390	С		A 181	-2.519	57.566	37.284	1.00100.00
15	15	ATOM	1391	0		A 181	-2.605	58.114	36.192	1.00100.00
10	15	ATOM	1392	CB		A 181	-1.014	57.340	39.210	1.00 92.48
		MOTA	1393	CG		A 181	-0.362	58.734	39.152	1.00 98.39
		MOTA	1394	CD		A 181	0.268	58.736	37.663	1.00 94.17
		ATOM ATOM	1395 1396	N CA		A 182 A 182	-3.567 -4.822	57.456	38.141	1.00100.00
	20	ATOM	1397	C		A 182	-5.359	58.161 58.856	37.876 39.154	1.00 98.21
	20	ATOM	1398	õ		A 182	-6.404	59.497	39.167	1.00100.00 1.00 99.44
20		ATOM	1399	СВ		A 182	-5.854	57.142	37.356	1.00 98.57
		ATOM	1400	CG		A 182	-5.880	57.077	35.816	1.00100.00
		ATOM	1401	CD		A 182	-7.013	57.938	35.300	1.00100.00
	25	ATOM	1402		GLU .		-7.817	58.385	36.105	1.00100.00
		ATOM	1403	OE2	GLU .	A 182	-7.084	58.153	34.091	1.00100.00
		ATOM	1404	N	ASP .	A 183	-4.607	58.672	40.265	1.00 98.63
25		ATOM	1405	CA	ASP.	A 183	-5.021	59.257	41.552	1.00 97.49
	••	ATOM	1406	С		A 183	-4.126	60.472	41.932	1.00100.00
	30	ATOM	1407	0		A 183	-3.464	61.061	41.079	1.00100.00
		ATOM	1408	CB		A 183	-4.946	58.144	42.619	1.00 98.36
		MOTA	1409	CG		A 183	-3.612	57.409	42.547	1.00100.00
		ATOM	1410		ASP .		-3.471	56.556	41.668	1.00100.00
20	35	ATOM	1411		ASP .		-2.741	57.688	43.364	1.00100.00
30	33	ATOM ATOM	1412 1413	N CA		A 184 A 184	-4.187	60.906	43.237	1.00 97.96
		ATOM	1414	C		A 184	-3.311 -1.865	61.985 61.528	43.738 44.071	1.00 97.92
		ATOM	1415	õ.		A 184	-1.348	61.748	45.159	1.00 97.89 1.00100.00
		ATOM	1416	СВ		A 184	-3.973	62.561	44.992	1.00100.00
	40	ATOM	1417	CG		A 184	-5.262	61.777	45.284	1.00100.00
		ATOM	1418	CD		A 184	-5.122	60.532	44.284	1.00 97.20
35		ATOM	1419	N	SER .	A 185	-1.249	60.840	43.071	1.00 82.40
		ATOM	1420	CA	SER .	A 185	0.196	60.496	43.086	1.00 75.26
	4.5	ATOM	1421	С	SER .	A 185	0.748	60.563	41.623	1.00 71.84
	45	ATOM	1422	0		A 185	-0.006	60.525	40.670	1.00 77.97
		ATOM	1423	CB		A 185	0.337	59.068	43.636	1.00 73.41
		ATOM	1424	OG		A 185	0.672	59.109	45.027	1.00 63.60
40		ATOM	1425	N		A 186	2.107	60.704	41.461	1.00 57.89
	50	ATOM ATOM	1426 1427	CA C		A 186	2.650	60.971	40.088	1.00 56.00
	50	ATOM	1428	ò		A 186 A 186	3.725	59.943	39.633	1.00 59.64
		ATOM	1429	СВ		A 186	4.473 3.258	60.157 62.393	38.688 40.064	1.00 60.30
		ATOM	1430	ĊG		A 186	2.339	63.457	40.677	1.00 63.74 1.00 80.44
		ATOM	1431	CD		A 186	1.188	63.874	39.736	1.00 71.31
45	55	ATOM	1432	NE		A 186	1.316	63.215	38.436	1.00 79.64
45		MOTA	1433	CZ		A 186	0.185	62.862	37.784	1.00 95.30
		ATOM	1434		ARG .		-0.999	63.109	38.312	1.00 56.25
		ATOM	1435		ARG .		0.276	62.232	36.603	1.00 89.98
		MOTA	1436	N		A 187	3.892	58.778	40.265	1.00 54.50
	60	ATOM	1437	CA	LYS .	A 187	4.891	57.805	39.851	1.00 51.93
		MOTA	1438	С		A 187	4.506	56.436	40.276	1.00 52.96
50		ATOM	1439	0		A 187	3.971	56.236	41.368	1.00 53.58
		ATOM	1440	CB		A 187	6.247	58.047	40.470	1.00 53.78
		ATOM	1441	CG	LYS .	A 187	7.427	57.714	39.574	1.00 43.05

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5		ATOM	1442	CD	LYS A 1	187	8.517	58.761	39.762	1.00 53.36
		ATOM	1443	CE	LYS A 1		9.870	58.468	39.146	1.00 39.68
		ATOM	1444	NZ	LYS A 1		10.795	59.601	39.341	1.00 40.19
		ATOM	1445	N	ILE A 1		4.819	55.502	39.403	1.00 46.36
	5	ATOM	1446	CA	ILE A 1		4.565	54.128	39.700	1.00 43.57
	_	ATOM	1447	C	ILE A 1		5.824	53.311	39.851	1.00 43.57
		ATOM	1448	ŏ	ILE A	198	6.647	53.189	38.937	
10		ATOM	1449	СВ	ILE A		3.579			1.00 41.55
		ATOM	1450		ILE A			53.425	38.826	1.00 45.64
	10	ATOM	1451				2.193	54.021	39.047	1.00 45.82
	10	ATOM	1452		ILE A 1		3.590	51.969	39.273	1.00 43.43
					ILE A 1		1.448	53.505	40.276	1.00 62.08
		ATOM	1453	N	TYR A 1		5.950	52.757	41.042	1.00 35.58
		ATOM	1454	CA	TYR A 1		7.079	51.933	41.356	1.00 37.57
15	15	ATOM	1455	C	TYR A 1		6.652	50.465	41.359	1.00 44.89
, •	13	ATOM	1456	0	TYR A 1		5.656	50.092	41.999	1.00 44.33
		ATOM	1457	СВ	TYR A 1		7.752	52.392	42.661	1.00 37.85
		ATOM	1458	CG	TYR A 1		8.692	53.563	42.456	1.00 34.49
		ATOM	1459		TYR A 1		9.968	53.375	41.930	1.00 35.93
	-00	ATOM	1460		TYR A 1		8.310	54.859	42.813	1.00 32.44
	20	ATOM	1461		TYR A 1		10.843	54.449	41.753	1.00 36.88
20		ATOM	1462	CE2	TYR A 1		9.170	55.945	42.647	1.00 31.63
20		ATOM	1463	CZ	TYR A 1	189	10.441	55.734	42.113	1.00 44.54
		ATOM	1464	OH	TYR A 1	189	11.296	56.788	41.929	1.00 57.77
		ATOM	1465	N	LYS A 1	190	7.413	49.651	40.608	1.00 42.91
	25	ATOM	1466	CA	LYS A 1	190	7.173	48.210	40.420	1.00 42.22
		ATOM	1467	С	LYS A 1	190	8.152	47.262	41.143	1.00 40.73
		ATOM	1468	0	LYS A 1	190	9.398	47.400	41.093	1.00 35.69
25		MOTA	1469	CB	LYS A 1	190	7.007	47.839	38.944	1.00 45.87
		ATOM	1470	CG	LYS A 1	190	5.735	48.403	38.306	1.00 71.08
	30	MOTA	1471	CD	LYS A 1	190	5.758	48.384	36.779	1.00 84.62
		ATOM	1472	CE	LYS A 1	190	4.386	48.157	36.147	1.00100.00
		ATOM	1473	NZ	LYS A 1	190	4.299	46.930	35.329	1.00100.00
		ATOM	1474	N	PHE A 1	191	7.539	46.264	41.812	1.00 35.01
		ATOM	1475	CA	PHE A 1		8.276	45.304	42.592	1.00 31.57
30	35	ATOM	1476	С	PHE A 1		7.792	43.871	42.465	1.00 30.89
		ATOM	1477	0	PHE A 1		6.603	43.584	42.377	1.00 25.06
		ATOM	1478	CB	PHE A 1		8.217	45.734	44.080	1.00 32.11
		ATOM	1479	CG	PHE A 1		8.570	47.190	44.372	1.00 29.24
		ATOM	1480	CD1	PHE A 1		9.895	47.593	44.539	1.00 31.81
	40	ATOM	1481		PHE A 1		7.565	48.147	44.508	1.00 30.17
		ATOM	1482		PHE A 1		10.230	48.925	44.805	1.00 34.10
35		ATOM	1483		PHE A 1		7.866	49.483	44.776	1.00 33.69
		ATOM	1484	CZ	PHE A 1		9.201	49.860	44.928	1.00 33.32
		ATOM	1485	N	ILE A 1		8.764	42.961	42.505	1.00 35.75
	45	ATOM	1486	CA	ILE A 1		8.525	41.520	42.415	1.00 37.02
		ATOM	1487	C	ILE A 1		9.255	40.653	43.469	1.00 37.02
		ATOM	1488	ō	ILE A 1		10.489	40.672	43.593	1.00 33.03
		ATOM	1489	СВ	ILE A 1		8.850	40.970	41.025	
40		ATOM	1490		ILE A 1		8.289	41.914		1.00 42.45
	50	ATOM	1491		ILE A 1		8.251		39.981	1.00 46.39
	-	ATOM	1492		ILE A 1		7.609	39.567	40.859	1.00 44.02
		ATOM	1493	N	GLN A 1			41.231	38.798	1.00 69.61
		ATOM	1494	CA			8.459	39.864	44.195	1.00 27.51
		ATOM	1495		GLN A 1		8.954	38.908	45.177	1.00 32.05
	55			C	GLN A 1		8.626	37.488	44.757	1.00 44.32
45	33	ATOM	1496	0	GLN A 1		7.583	36.926	45.120	1.00 43.11
		ATOM	1497	CB	GLN A 1		8.502	39.100	46.638	1.00 33.44
		ATOM	1498	CG	GLN A 1		9.285	38.203	47.632	1.00 22.34
		ATOM	1499	CD	GLN A·1		10.824	38.337	47.636	1.00 48.52
	60	MOTA	1500		GLN A 1		11.557	37.537	47.016	1.00 45.24
	60	MOTA	1501		GLN A 1		11.326	39.330	48.373	1.00 24.82
		ATOM	1502	N	LYS A 1		9.543	36.908	43.993	1.00 46.91
50		MOTA	1503	CA	LYS A 1		9.384	35.540	43.529	1.00 47.56
		ATOM	1504	C	LYS A 1		9.456	34.524	44.666	1.00 49.56
		ATOM	1505	0	LYS A 1	.94	8.777	33.520	44.598	1.00 50.85

5		ATOM	1506	CB	LYS A 194	10.385	35.159	42.439	1.00 48.11
		ATOM	1507	CG	LYS A 194	9.884	35.443	41.031	1.00 55.70
		ATOM	1508	CD	LYS A 194	10.895	36.200	40.179	1.00 67.67
		ATOM	1509	CE	LYS A 194	10.614	36.122	38.682	1.00 81.92
	5	ATOM	1510	NZ	LYS A 194	11.284	37.185	37.910	1.00 88.34
		ATOM	1511	N	VAL A 195	10.308	34.753	45.689	1.00 39.55
		ATOM	1512	CA	VAL A 195	10.422	33.780	46.764	1.00 33.56
10		ATOM	1513	C	VAL A 195	9.261	33.862	47.698	1.00 35.67
		ATOM	1514	ŏ	VAL A 195	8.804	34.945	48.034	
	10	ATOM	1515	СВ	VAL A 195	11.716	33.844	47.560	1.00 38.69 1.00 32.62
	••	ATOM	1516		VAL A 195	11.849	32.539	48.310	
		ATOM	1517		VAL A 195	12.933	34.029		1.00 32.40
		ATOM	1518	N	PRO A 196	8.770		46.667	1.00 30.55
		ATOM	1519	CA	PRO A 196		32.717	48.126	1.00 27.75
15	15	ATOM	1520	C		7.653	32.757	49.038	1.00 26.18
	13				PRO A 196	8.132	33.236	50.410	1.00 35.86
		ATOM	1521	0	PRO A 196	9.185	32.809	50.899	1.00 35.43
		ATOM	1522	CB	PRO A 196	7.022	31.359	49.044	1.00 26.04
		ATOM	1523	CG	PRO A 196	7.856	30.472	48.113	1.00 27.79
	20	ATOM	1524	CD	PRO A 196	8.964	31.352	47.546	1.00 25.40
	20	ATOM	1525	N	ILE A 197	7.388	34.171	51.009	1.00 29.92
20		ATOM	1526	CA	ILE A 197	7.772	34.697	52.284	1.00 26.98
20		ATOM	1527	С	ILE A 197	6.544	34.809	53.128	1.00 34.88
		ATOM	1528	0	ILE A 197	5.444	34.788	52.606	1.00 29.68
		ATOM	1529	СВ	ILE A 197	8.334	36.100	52.094	1.00 27.90
	25	ATOM	1530		ILE A 197	7.342	36.867	51.254	1.00 27.78
		ATOM	1531		ILE A 197	9.659	36.091	51.337	1.00 28.12
		ATOM	1532		ILE A 197	7.494	38.378	51.438	1.00 28.12
25		ATOM	1533	N	PRO A 198	6.743			
25		ATOM	1534	CA	PRO A 198		34.936	54.447	1.00 36.02
	30	ATOM	1535			5.647	35.110	55.410	1.00 31.31
	50			C	PRO A 198	5.299	36.583	55.308	1.00 28.27
		ATOM	1536	0	PRO A 198	6.212	37.391	55.115	1.00 22.70
		MOTA	1537	CB	PRO A 198	6.252	34.849	56.794	1.00 31.17
		ATOM	1538	CG	PRO A 198	7.768	34.768	56.615	1.00 34.94
	25	ATOM	1539	CD	PRO A 198	8.057	34.706	55.122	1.00 32.99
30	35	ATOM	1540	N	CYS A 199	4.011	36.939	55.405	1.00 27.60
		ATOM	1541	CA	CYS A 199	3.555	38.360	55.289	1.00 27.66
		ATOM	1542	С	CYS A 199	4.255	39.390	56.187	1.00 30.13
		ATOM	1543	0	CYS A 199	4.294	40.596	55.895	1.00 29.50
		ATOM	1544	CB	CYS A 199	2.025	38.534	55.242	1.00 27.18
	40	ATOM	1545	SG	CYS A 199	1.232	38.279	56.841	1.00 30.85
0.		ATOM	1546	N	TYR A 200	4.847	38.903	57.270	1.00 26.15
35		ATOM	1547	CA	TYR A 200	5.538	39.798	58.123	1.00 28.28
		ATOM	1548	С	TYR A 200	6.760	40.395	57.483	1.00 32.29
		ATOM	1549	0	TYR A 200	7.359	41.286	58.036	1.00 31.56
	45	ATOM	1550	СВ	TYR A 200	5.844	39.215	59.489	1.00 31.30
		ATOM	1551	CG	TYR A 200	6.989	38.272		
		ATOM	1552		TYR A 200	8.288		59.568	1.00 28.28
		ATOM	1553		TYR A 200		38.733	59.689	1.00 29.48
40		ATOM	1554			6.756	36.903	59.475	1.00 27.55
	50		1555		TYR A 200	9.377	37.862	59.825	1.00 21.42
	50	ATOM			TYR A 200	7.838	36.015	59.595	1.00 27.41
		ATOM	1556	CZ	TYR A 200	9.144	36.488	59.737	1.00 25.11
		MOTA	1557	OH	TYR A 200	10.215	35.614	59.880	1.00 27.62
		MOTA	1558	N	LEU A 201	7.113	39.897	56.313	1.00 31.66
		ATOM	1559	CA	LEU A 201	8.278	40.378	55.579	1.00 29.49
45	55	MOTA	1560	C	LEU A 201	7.914	41.343	54.484	1.00 33.65
		MOTA	1561	0	LEU A 201	8.767	41.737	53.686	1.00 35.31
		MOTA	1562	CB	LEU A 201	9.225	39.275	55.035	1.00 27.04
		MOTA	1563	CG	LEU A 201	9.697	38.271	56.071	1.00 27.42
		MOTA	1564		LEU A 201	10.254	37.030	55.390	1.00 23.71
	60	ATOM	1565		LEU A 201	10.764	38.913	56.957	1.00 30.55
		ATOM	1566	N	ILE A 202	6.648	41.710		
50		MOTA	1567	CA	ILE A 202	6.249		54.438	1.00 28.66
55		MOTA	1568				42.674	53.433	1.00 29.57
				C	ILE A 202	6.636	44.074	53.951	1.00 40.28
		MOTA	1569	0	ILE A 202	6.192	44.493	55.027	1.00 40.75

5		ATOM	1570	CB	ILE A 202	4.733	42.651	53.182	1.00 31.18
		MOTA	1571	CG1	ILE A 202	4.250	41.429	52.405	1.00 28.21
		ATOM	1572	CG2	ILE A 202	4.259	43.962	52.521	1.00 29.23
		ATOM	1573	CD1	ILE A 202	2.724	41.288	52.449	1.00 23.01
	5	MOTA	1574	N	ALA A 203	7.445	44.813	53.197	1.00 39.14
		ATOM	1575	CA	ALA A 203	7.840	46.150	53.611	1.00 37.03
		ATOM	1576	Ç	ALA A 203	7.819	47.159	52.482	1.00 34.32
10		ATOM	1577	ō	ALA A 203	8.060	46.836	51.311	1.00 30.63
		ATOM	1578	СВ	ALA A 203	9.180	46.143	54.309	1.00 30.03
	10	ATOM	1579	N	LEU A 204	7.514	48.388	52.910	
		ATOM	1580	CA	LEU A 204	7.388	49.604		1.00 33.64
		ATOM	1581	c	LEU A 204			52.102	1.00 32.56
		ATOM	1582			7.993	50.817	52.812	1.00 37.69
				0	LEU A 204	7.854	51.037	54.034	1.00 32.66
15	15	ATOM	1563	CB	LEU A 204	5.906	49.929	51.718	1.00 29.74
, •	15	ATOM	1584	CG	LEU A 204	5.706	51.182	50.855	1.00 29.64
		ATOM	1585		LEU A 204	6.263	50.994	49.445	1.00 29.47
		ATOM	1586		LEU A 204	4.222	51.515	50.750	1.00 33.50
		ATOM	1587	N	VAL A 205	8.670	51.603	51.991	1.00 36.87
	20	ATOM	1588	CA	VAL A 205	9.305	52.821	52.415	1.00 35.15
	20	ATOM	1589	С	VAL A 205	9.224	53.795	51.284	1.00 38.41
20		ATOM	1590	0	VAL A 205	9.575	53.462	50.148	1.00 39.50
20		ATOM	1591	CB	VAL A 205	10.769	52.651	52,804	1.00 36.06
		ATOM	1592	CG1	VAL A 205	11.466	51.794	51.757	1.00 35.08
		ATOM	1593	CG2	VAL A 205	11.432	54.020	52.833	1.00 35.98
	25	ATOM	1594	N	VAL A 206	8.750	54.983	51.623	1.00 33.54
		ATOM	1595	CA	VAL A 206	8.623	56.104	50.687	1.00 31.81
		ATOM	1596	С	VAL A 206	9.300	57.343	51.249	1.00 31.62
25		ATOM	1597	Ó	VAL A 206	9.076	57.722	52.406	1.00 34.81
25		ATOM	1598	СВ	VAL A 206	7.179	56.405	50.305	1.00 33.35
	30	ATOM	1599		VAL A 206	7.129	57.243	49.029	1.00 33.33
		ATOM	1600		VAL A 206	6.452	55.084	50.109	1.00 31.98
		ATOM	1601	N	GLY A 207	10.130	57.959	50.431	1.00 31.90
		ATOM	1602	CA	GLY A 207	10.807	59.168	50.861	1.00 27.25
		ATOM	1603	c c	GLY A 207	11.802	59.632	49.838	1.00 38.81
30	35	ATOM	1604	ō	GLY A 207	12.046	58.966	48.840	1.00 30.81
50		ATOM	1605	N	ALA A 208	12.375	60.783	50.113	
		ATOM	1606	CA	ALA A 208	13.370	61.354	49.233	1.00 41.07
		MOTA	1607	c	ALA A 208	14.660	60.550		1.00 42.72
		ATOM	1608	Ö	ALA A 208			49.356	1.00 49.10
	40	ATOM	1609	СВ		15.651	60.997	49.957	1.00 51.30
	40	ATOM	1610		ALA A 208	13.605	62.810	49.589	1.00 42.95
35				N	LEU A 209	14.623	59.350	48.773	1.00 40.92
••		ATOM	1611	CA	LEU A 209	15.739	58.440	48.825	1.00 39.55
		ATOM	1612	C	LEU A 209	16.756	58.575	47.743	1.00 47.96
	45	ATOM	1613	0	LEU A 209	16.420	58.843	46.597	1.00 49.44
	43	ATOM	1614	CB	LEU A 209	15.269	56.994	48.894	1.00 37.97
		ATOM	1615	CG	LEU A 209	14.420	56.803	50.129	1.00 40.46
		MOTA	1616		LEU A 209	13.713	55.469	50.075	1.00 36.99
40		ATOM	1617		LEU A 209	15.283	56.921	51.387	1.00 43.31
10	50	MOTA	1618	N	GLU A 210	17.999	58.317	48.182	1.00 42.68
	50	MOTA	1619	CA	GLU A 210	19.205	58.311	47.381	1.00 40.30
		MOTA	1620	С	GLU A 210	19.965	57.056	47.693	1.00 47.51
		MOTA	1621	0	GLU A 210	19.708	56.432	48.721	1.00 47.89
		MOTA	1622	CB	GLU A 210	20.084	59.553	47.613	1.00 42.01
		ATOM	1623	CG	GLU A 210	19.699	60.734	46.697	1.00 58.26
45	55	ATOM	1624	CD	GLU A 210	20.524	61.970	46.897	1.00100.00
40		MOTA	1625		GLU A 210	21.629	61.968	47.451	1.00 95.26
		ATOM	1626	OE2	GLU A 210	19.935	63.047	46.486	1.00100.00
		ATOM	1627	N	SER A 211	20.895	56.662	46.805	
		MOTA	1628	CA	SER A 211	21.661			1.00 45.01
	60	ATOM	1629	C			55.442	47.013	1.00 42.25
	50				SER A 211	23.143	55.535	46.667	1.00 43.37
50		MOTA	1630	O	SER A 211	23.649	56.493	46.086	1.00 46.43
50		MOTA	1631	CB	SER A 211	21.025	54.233	46.346	1.00 44.33
		ATOM	1632	OG	SER A 211	21.274	54.244	44.934	1.00 54.15
		ATOM	1633	N	ARG A 212	23.829	54.497	47.053	1.00 34.85

5		ATOM	1634	CA	ARG .	A 2	212	25.229	54.328	46.791	1.00 35.41
		ATOM	1635	С	ARG .	A 2	212	25.430	52.838	46.567	1.00 45.39
		ATOM	1636	0	ARG .	A 2	212	24.840	52.027	47.276	1.00 48.85
	_	MOTA	1637	CB	ARG .	A 2	212	26.101	54.846	47.915	1.00 37.25
	5	ATOM	1638	CG	ARG .	A 2	212	27.151	55.827	47.402	1.00 68.10
		ATOM	1639	CD .	ARG .	A 2	212	26.532	56.962	46.587	1.00 76.55
		ATOM	1640	NE	ARG .			26.695	58.307	47.148	1.00 55.19
10		ATOM	1641	CZ	ARG .			25.845	59.301	46.867	1.00 70.87
		ATOM	1642	NH1	ARG .			24.806	59.105	46.059	1.00 35.71
	10	ATOM	1643		ARG .			26.032	60.516	47.392	1.00 73.35
		ATOM	1644	N	GLN			26.210	52.442	45.567	1.00 40.74
		ATOM	1645	CA	GLN .			26.408	51.021	45.331	1.00 39.90
		ATOM	1646	C	GLN .			27.646	50.537	46.050	1.00 39.90
		ATOM	1647	ō	GLN .			28.740	50.981	45.741	1.00 53.77
15	15	ATOM	1648	CB	GLN .			26.545	50.741	43.846	1.00 40.99
		ATOM	1649	CG	GLN .			26.976	49.296	43.532	1.00 55.79
		ATOM	1650	CD	GLN			26.292	48.743	42.301	
		ATOM	1651		GLN .			26.275	47.523	42.102	1.00 76.04
		ATOM	1652	NE2	GLN .			25.700	49.618		1.00 86.66
	20	ATOM	1653	N	ILE .			27.495		41.489	1.00 55.45
	LU	ATOM	1654	CA					49.649	47.013	1.00 33.12
20		ATOM	1655	C	ILE .			28.663	49.206	47.743	1.00 32.55
					ILE .			28.911	47.765	47.536	1.00 39.29
		MOTA MOTA	1656	0	ILE .			29.726	47.162	48.230	1.00 42.41
	25		1657	CB	ILE .			28.546	49.428	49.250	1.00 35.72
	23	ATOM	1658		ILE .			27.395	48.573	49.791	1.00 36.13
		ATOM	1659		ILE /			28.344	50.911	49.598	1.00 35.79
		ATOM	1660		ILE .			27.067	48.841	51.260	1.00 46.69
25		ATOM	1661	N	GLY .			28.199	47.197	46.598	1.00 35.02
	20	ATOM	1662	CA	GLY :			28.638	45.855	46.234	1.00 34.88
	30	ATOM	1663	С	GLY .			27.970	45.405	44.950	1.00 41.09
		MOTA	1664	0	GLY .	A 2	215	27.083	46.048	44.425	1.00 44.25
		ATOM	1665	N	PRO .	A 2	216	28.448	44.262	44.410	1.00 39.62
		MOTA	1666	CA	PRO .	A 2	216	27.890	43.720	43.197	1.00 39.69
		ATOM	1667	С	PRO .	A 2	216	26.369	43.661	43.253	1.00 41.56
30	35	ATOM	1668	0	PRO .	A 2	216	25.655	43.817	42.240	1.00 44.35
		ATOM	1669	CB	PRO .	A 2	216	28.448	42.311	42.996	1.00 39.91
		ATOM	1670	CG	PRO A	A 2	216	29.377	41.993	44.164	1.00 41.54
		ATOM	1671	CD	PRO 2	A 2	216	29.514	43.411	44.897	1.00 37.70
		ATOM	1672	N	ARG .	A 2	217	25.846	43.398	44.477	1.00 31.04
	40	ATOM	1673	CA	ARG A	A 2	217	24.421	43.328	44.652	1.00 29.22
Ω		ATOM	1674	С	ARG A			23.928	44.109	45.872	1.00 38.24
35		ATOM	1675	0	ARG A			22.861	43.885	46.368	1.00 40.69
		ATOM	1676	СВ	ARG 2	A 2	217	24.012	41.844	44.790	1.00 22.75
		ATOM	1677	CG	ARG A			25.221	40.963	45.109	1.00 40.77
	45	ATOM	1678	CD	ARG .			24.828	39.774	45.985	1.00 34.08
		ATOM	1679	NE	ARG A			26.020	39.183	46.581	1.00 45.20
		ATOM	1680	CZ	ARG A			25.955	37.894	46.911	1.00 65.13
		ATOM	1681		ARG Z			24.832	37.220	46.716	1.00 42.40
40		ATOM	1682		ARG .			26.997	37.300	47.472	1.00 48.08
	50	ATOM	1683	N	THR .			24.784	45.022	46.404	1.00 31.00
		ATOM	1684	CA	THR 2			24.309	45.886	47.487	
		ATOM	1685	c	THR I			24.128	47.319		1.00 31.00
		ATOM	1686	ŏ	THR					47.021	1.00 43.60
		ATOM	1687	СВ	THR I			25.065	47.930	46.512	1.00 48.42
	55	ATOM						25.315	45.845	48.640	1.00 36.95
45			1688		THR A			25.430	44.517	49.139	1.00 45.66
		ATOM	1689		THR A			24.826	46.751	49.766	1.00 34.17
		ATOM	1690	N	LEU A			23.099	48.018	47.431	1.00 39.19
		ATOM	1691	CA	LEU Z			23.055	49.452	47.315	1.00 38.18
	<i>(</i> 0	ATOM	1692	С	LEU Z			22.713	50.000	48.695	1.00 42.32
	60	ATOM	1693	O	LEU A			22.108	49.289	49.498	1.00 43.67
		ATOM	1694	CB	LEU A			21.927	49.841	46.356	1.00 37.05
50		ATOM	1695	CG	LEU A			22.386	50.657	45.168	1.00 39.31
		ATOM	1696	CD1	LEU A	A 2	219	23.670	50.064	44.613	1.00 40.57
		ATOM	1697		LEU A			21.283	50.619	44.131	1.00 29.39

5		ATOM	1698	N	VAL	А	220	23.066	51.241	48.976	1 00	35.01
_		ATOM	1699	CA			220	22.741	51.830	50.253		36.98
		MOTA	1700	C	VAL			21.736	52.923	50.043		44.08
		MOTA	1701	0			220	21.959	53.835	49.256		46.60
	5	MOTA	1702	CB	VAL	A	220	23.965	52.346	51.028		44.95
		MOTA	1703	CG1	VAL	Α	220	23.675	52.428	52.516		43.16
		ATOM	1704	CG2	VAL	A	220	25.138	51.382	50.828		47.70
10		MOTA	1705	N	TRP	A	221	20.622	52.818	50.731		41.98
		MOTA	1706	CA	TRP	Α	221	19.605	53.828	50.602		41.64
	10	MOTA	1707	С	TRP	A	221	19.464	54.612	51.872		42.40
		MOTA	1708	0			221	19.461	54.060	52.960	1.00	45.56
		ATOM	1709	CB	TRP			18.256	53.245	50.186	1.00	41.24
		ATOM	1710	CG	TRP			18.353	52.459	48.918	1.00	42.59
15	1.5	MOTA	1711		TRP			18.888	51.225	48.793	1.00	45.35
,5	15	ATOM	1712		TRP			17.949	52.873	47.590	1.00	41.62
		ATOM	1713		TRP			18.826	50.832	47.478	1.00	44.74
		ATOM	1714		TRP			18.243	51.821	46.720		45.31
		ATOM	1715		TRP			17.345	54.009	47.061		41.17
	20	ATOM	1716		TRP			17.958	51.902	45.346		42.60
	20	ATOM ATOM	1717 1718		TRP TRP			17.054	54.083	45.710		39.08
20		ATOM	1719					17.360	53.040	44.864		38.48
		ATOM	1720	N	SER			19.271	55.896	51.688		37.01
		ATOM	1721	CA C	SER SER			19.017	56.846	52.748		38.05
	25	ATOM	1722	Ö				18.853	58.251	52.205		45.28
	20	ATOM	1723	CB	SER SER			19.005	58.503	51.008		44.02
		ATOM	1724	OG	SER			20.098	56.816	53.820		39.07
25		ATOM	1725	N	GLU			18.586	57.149 59.190	53.229		42.36
25		ATOM	1726	CA	GLU			18.465	60.527	53.088 52.584		40.91
	30	ATOM	1727	c	GLU			19.843	61.042	52.234		41.97
		ATOM	1728	ŏ	GLU			20.829	60.701	52.863		52.02
		ATOM	1729	СВ	GLU			17.856	61.483	53.597		43.06
		ATOM	1730	CG	GLU			16.364	61.262	53.861		51.71
		ATOM	1731	CD	GLU			15.799	62.478	54.545		84.51
30	35	MOTA	1732	OE1	GLU			15.905	63.610	54.085		56.82
		ATOM	1733	OE2	GLU	Α	223	15.244	62.222	55.705		88.87
		ATOM	1734	N	LYS	Α	224	19.892	61.875	51.229		47.39
		ATOM	1735	CA	LYS	Α	224	21.139	62.456	50.792		48.51
	4.0	MOTA	1736	C	LYS	Α	224	22.163	62.683	51.930		50.90
	40	ATOM	1737	0	LYS	Α	224	23.382	62.569	51.736		51.55
05		MOTA	1738	CB	LYS	Α	224	20.843	63.736	49.986	1.00	51.58
35		ATOM	1739	CG	LYS	А	224	22.039	64.648	49.723	1.00	81.16
		MOTA	1740	CD	LYS			21.954	65.397	48.392	1.00	97.82
	A.E.	ATOM	1741	CE	LY5			21.646	66.891	48.530	1.001	00.00
	45	MOTA	1742	NZ	LYS			22.056	67.700	47.362	1.001	00.00
		ATOM	1743	N	GLU			21.683	63.011	53.123	1.00	45.77
		ATOM	1744	CA	GLU			22.607	63.309	54.199		46.00
40		ATOM	1745	C	GLU			23.227	62.150	54.902		47.99
	50	ATOM	1746	0	GLU			24.107	62.354	55.732		47.21
	50	ATOM	1747	CB	GLU			22.057	64.296	55.210		47.71
		ATOM	1748	CG	GLU				64.296	55.182		63.24
		ATOM	1749	CD	GLU			19.931	65.219	54.150		75.13
		ATOM ATOM	1750 1751		GLU			20.187	66.420	54.046		54.64
	55	ATOM	1752	N N	GLU			19.039 22.798	64.578	53.420		49.64
45	55	ATOM	1753	CA	GLN GLN			23.340	60.949	54.564		43.92
		ATOM	1754	c	GLN				59.772	55.224		43.91
		ATOM	1755	0	GLN			24.036 24.756	58.756 57.871	54.322		45.86
		ATOM	1756	СВ	GLN			22.252	59.084	54.806 56.063		45.70
	60	ATOM	1757	CG	GLN			21.965	59.790	57.400		45.27
		ATOM	1758	ÇD	GLN			21.297	61.155	57.302		31.17
50		ATOM	1759		GLN			21.823	62.149	57.820		37.36
		ATOM	1760		GLN			20.115	61.202	56.696		30.28
		ATOM	1761	N	VAL			23.814	58.871	53.021		41.20
					_				50.011	55.021	1.00	-+,20

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5		ATOM	1762	CA	VAL				.406	57.947	52.071	1.00 43.13
		ATOM	1763	С	VAL				.884	57.670	52.261	1.00 50.55
		ATOM	1764	0	VAL				.298	56.518	52.480	1.00 53.01
		ATOM	1765	CB	VAL				.155	58.293	50.604	1.00 49.39
	5	ATOM	1766		VAL				.319	57.029	49.771	1.00 48.89
		ATOM	1767		VAL				.752	58.851	50.421	1.00 50.47
10		ATOM	1768	N	GLU				.696	58.718	52.170	1.00 44.08
10		ATOM	1769	CA	GLU				.123	58.542	52.310	1.00 41.71
	10	ATOM	1770	С	GLU				.514	57.871	53.583	1.00 44.20
	10	ATOM	1771	0	GLU				.227	56.868	53.589	1.00 44.88
		ATOM	1772	CB	GLU				.935	59.824	52.102	1.00 43.08
		ATOM	1773	CG	GLU				.153	60.161	50.611	1.00 64.74
		ATOM	1774	CD	GLU				.114	58.965	49.701	1.00 84.29
15	15	ATOM	1775		GLU				.975	58.107	49.685	1.00 84.36
, -	13	ATOM	1776		GLU				.064	58.951	48.917	1.00 73.81
		ATOM	1777	N	LYS				.066	58.423	54.685	1.00 39.79
		ATOM	1778	CA	LYS				.449	57.796	55.922	1.00 39.04
		ATOM	1779	C	LYS				.949	56.375	55.930	1.00 40.38
	20	ATOM	1780	O	LYS				.639	55.433	56.346	1.00 43.63
	20	ATOM	1781	CB	LYS				.129	58.585	57.187	1.00 39.79
20		ATOM	1782 1783	CG	LYS				.903	58.072	58.394	1.00 63.75
		ATOM	1784	CD	LYS				.498	58.763	59.685	1.00 77.46
		ATOM ATOM	1785	CE NZ	LYS				.677	59.084	60.593	1.00 94.73
	25	ATOM	1786	N Z	LYS				.344	60.353	60.256	1.00100.00
	23	ATOM	1787		SER				.741	56.220	55.428	1.00 28.48
		ATOM	1788	CA C	SER				.174	54.891	55.377	1.00 25.93
		MOTA	1789	0	SER				.089	53.988	54.587	1.00 30.26
25		ATOM	1790		SER				.469	52.855	54.955	1.00 28.48
	30		1791	CB	SER				.824	54.927	54.694	1.00 30.08
	50	ATOM ATOM	1792	OG N	SER				.822	55.293	55.605	1.00 41.60
		ATOM	1793	n Ca	ALA ALA				.436	54.536	53.459	1.00 31.13
		ATOM	1794	C	ALA				.288	53.820	52.593	1.00 36.66
		ATOM	1795	ŏ	ALA				.597 .003	53.383	53.270	1.00 47.68
30	35	ATOM	1796	СВ	ALA				.406	52.238 54.518	53.103	1.00 54.59
50	50	ATOM	1797	N	TYR				.256	54.246	51.257 54.060	1.00 38.49
		ATOM	1798	CA	TYR				.500	53.830	54.730	1.00 40.77
		ATOM	1799	c	TYR				.265	52.721	55.753	1.00 38.40 1.00 39.70
		ATOM	1800	ō	TYR				.041	51.772	55.862	1.00 36.46
	40	ATOM	1801	СВ	TYR				.311	54.981	55.414	1.00 38.46
		ATOM	1802	CG	TYR				.497	54.525	56.303	1.00 38.27
35		ATOM	1803		TYR				.755	54.238	55.753	1.00 46.41
		ATOM	1804		TYR				.373	54.394	57.691	1.00 40.99
		ATOM	1805		TYR				.835	53.815	56.534	1.00 47.23
	45	ATOM	1806		TYR				.441	53.979	58.496	1.00 40.10
		ATOM	1807	CZ	TYR				.680	53.695	57.916	1.00 48.59
		MOTA	1808	OH	TYR				.734	53.282	58.698	1.00 51.92
40		ATOM	1809	N	GLU				.191	52.883	56.519	1.00 35.75
40		ATOM	1810	CA	GLU				.835	51.984	57.606	1.00 34.55
	50	ATOM	1811	С	GLU				.633	50.498	57.252	1.00 38.39
		ATOM	1812	0	GLU	Α	233		.152	49.576	57.892	1.00 38.55
		ATOM	1813	CB	GLU	Α	233	28	.673	52.623	58.414	1.00 34.48
		ATOM	1814	CG	GLU	A	233		.666	52.262	59.912	1.00 24.95
		MOTA	1815	CD	GLU	Α	233	29	.463	53.183	60.787	1.00 37.55
45	55	MOTA	1816	OE1	GLU	Α	233	29	.408	54.410	60.741	1.00 55.33
• •		ATOM	1817	OE2	GLU	Α	233	30	.216	52.518	61.619	1.00 40.65
		MOTA	1818	N	PHE	A	234		.867	50.282	56.202	1.00 33.02
		ATOM	1819	CA	PHE				. 493	48.974	55.719	1.00 29.90
		ATOM	1820	C	PHE				.341	48.398	54.592	1.00 34.69
	60	ATOM	1821	0	PHE			28	.883	47.521	53.823	1.00 34.21
		ATOM	1822	CB	PHE				.020	49.081	55.293	1.00 30.23
50		MOTA	1823	CG	PHE	Α	234		.215	49.752	56.394	1.00 30.32
		ATOM	1824		PHE			26	.518	49.521	57.739	1.00 31.50
•		MOTA	1825	CD2	PHE	Α	234		.151	50.605	56.102	1.00 28.66
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5		ATOM	1826	CE1	PHE A	234	25.780	50.103	58.772	1.00 30.43
		ATOM	1827	CE2	PHE A		24.407	51.203	57.121	1.00 29.60
		MOTA	1828	CZ	PHE A		24.725	50.959	58.458	1.00 27.47
	_	MOTA	1829	N	SER A	235	30.571	48.874	54.476	1.00 29.55
	5	MOTA	1830	CA	SER A	235	31.428	48.366	53.412	1.00 28.64
		ATOM	1831	С	SER A	235	31.387	46.858	53.338	1.00 30.38
40		MOTA	1832	0	SER A	235	31.166	46.252	52.282	1.00 32.37
10		MOTA	1833	CB	SER A		32.861	48.787	53.604	1.00 31.15
	10	ATOM	1834	OG	SER A		33.028	49.368	54.873	1.00 39.32
	10	ATOM	1835	N	GLU A		31.698	46.299	54.504	1.00 22.49
		ATOM	1836	CA	GLU A		31.815	44.873	54.737	1.00 23.79
		ATOM	1837	Ç	GLU A		30.627	43.992	54.380	1.00 32.37
		ATOM	1838	0	GLU A		30.697	42.772	54.545	1.00 29.91
15	15	ATOM	1839	CB	GLU A		32.305	44.529	56.134	1.00 24.06
	13	ATOM	1840	CG	GLU A		33.491	45.403	56.585	1.00 22.96
		ATOM ATOM	1841 1842	CD OE1	GLU A		33.600	45.492	58.090	1.00 66.18
		ATOM	1843	OE2	GLU A		32.633	45.482	58.849	1.00 37.01
		ATOM	1844	N N	GLU A THR A		34.848 29.560	45.518	58.494	1.00 78.68
	20	ATOM	1845	CA	THR A		28.384	44.593	53.891	1.00 34.11
Ω	20	ATOM	1846	C	THR A		28.644	43.823 42.609	53.539 52.644	1.00 33.69
20		ATOM	1847	ŏ	THR A		28.517	41.451	53.048	1.00 33.33
		ATOM	1848	СВ	THR A		27.218	44.710	53.057	1.00 31.09 1.00 37.99
		ATOM	1849		THR A		26.899	45.675	54.048	1.00 37.99
	25	ATOM	1850		THR A		25.995	43.862	52.744	1.00 25.66
		ATOM	1851	N	GLU A		29.020	42.854	51.409	1.00 29.69
		ATOM	1852	CA	GLU A		29.267	41.734	50.520	1.00 27.05
25		ATOM	1853	С	GLU A		30.071	40.638	51.146	1.00 33.17
		ATOM	1854	0	GLU A		29.660	39.497	51.055	1.00 38.50
	30	ATOM	1855	CB	GLU A	238	29.851	42.080	49.161	1.00 27.50
		MOTA	1856	CG	GLU A	238	30.116	40.813	48.320	1.00 18.83
		MOTA	1857	CD	GLU A	238	28.902	40.297	47.596	1.00 41.67
		ATOM	1858	OE1	GLU A	238	27.848	40.909	47.464	1.00 33.59
		MOTA	1859	OE2	GLU A	238	29.085	39.089	47.138	1.00 46.30
30	35	MOTA	1860	N	SER A	239	31.203	40.973	51.772	1.00 24.44
		ATOM	1861	CA	SER A		32.045	39.957	52.387	1.00 24.60
		ATOM	1862	С	SER A		31.245	39.060	53.344	1.00 35.72
		ATOM	1863	0	SER A		31.379	37.830	53.360	1.00 35.25
	40	ATOM	1864	CB	SER A		33.231	40.601	53.074	1.00 29.14
	40	ATOM	1865	OG	SER A		32.747	41.590	53.961	1.00 54.60
35		ATOM	1866	N	MET A		30.382	39.703	54.154	1.00 33.13
		MOTA	1867	CA	MET A		29.529	38.993	55.091	1.00 28.55
		ATOM ATOM	1868 1869	C	MET A		28.603	38.075	54.325	1.00 35.65
	45	ATOM	1870	O CB	MET A		28.435	36.926	54.689	1.00 35.99
	15	ATOM	1871	CG	MET A		28.736 29.691	39.945	55.993	1.00 26.50
		ATOM	1872	SD	MET A		28.871	40.675 41.986	56.910 57.833	1.00 27.57
		ATOM	1873	CE	MET A		30.040			1.00 32.91
40		ATOM	1874	N	LEU A		28.019	42.085 38.603	59.183 53.243	1.00 28.47 1.00 32.77
	50	ATOM	1875	CA	LEU A		27.120	37.859	52.381	1.00 32.77
		ATOM	1876	c.	LEU A		27.848	36.615	51.878	1.00 25.07
		ATOM	1877	ō	LEU A		27.302	35.509	51.858	1.00 36.70
		ATOM	1878	СВ	LEU A		26.715	38.753	51.196	1.00 29.71
		ATOM	1879	CG	LEU A		25.283	39.289	51.237	1.00 37.68
45	55	ATOM	1880		LEU A		25.174	40.552	50.389	1.00 35.76
75		ATOM	1881		LEU A		24.309	38.257	50.673	1.00 45.60
		ATOM	1882	N	LYS A		29.114	36.806	51.468	1.00 34.76
		ATOM	1883	CA	LYS A		29.908	35.702	50.972	1.00 33.62
		ATOM	1884	С	LYS A		30.072	34.690	52.039	1.00 32.18
	60	ATOM	1885	0	LYS A		29.887	33.512	51.795	1.00 32.56
		ATOM	1886	CB	LYS A		31.292	36.069	50.468	1.00 38.43
50		ATOM	1887	CG	LYS A	242	31.406	36.263	48.961	1.00 49.23
		ATOM	1888	CD	LYS A		31.160	37.721	48.536	1.00 88.36
		ATOM	1889	CE	LYS A	242	32.371	38.456	47.943	1.00100.00

5		MOTA	1890	NZ	LYS A 242	32.033	39.411	46.862	1.00100.00
		ATOM	1891	N	ILE A 243	30.428	35.154	53.227	1.00 30.87
		MOTA	1892	CA	ILE A 243	30.627	34.229	54.359	1.00 31.70
	_	ATOM	1893	С	ILE A 243	29.381	33.458	54.764	1.00 36.50
	5	MOTA	1894	0	ILE A 243	29.458	32.303	55.119	1.00 39.33
		MOTA	1895	CB	ILE A 243	31.227	34.886	55.579	1.00 32.36
		MOTA	1896		ILE A 243	32.630	35.337	55.222	1.00 32.09
10		ATOM	1897	CG2	ILE A 243	31.243	33.891	56.718	1.00 28.26
		MOTA	1898	CD1	ILE A 243	33.035	36.578	55.981	1.00 20.09
	10	MOTA	1899	N	ALA A 244	28.237	34.120	54.708	1.00 32.10
		MOTA	1900	CA	ALA A 244	26.968	33.519	55.066	1.00 32.95
		ATOM	1901	С	ALA A 244	26.600	32.392	54.127	1.00 36.35
		MOTA	1902	0	ALA A 244	26.074	31.358	54.546	1.00 36.88
15	1.5	MOTA	1903	СВ	ALA A 244	25.858	34.576	55.123	1.00 34.02
,,	15	ATOM	1904	N	GLU A 245	26.890	32.617	52.846	1.00 31.20
		MOTA	1905	CA	GLU A 245	26.614	31.635	51.818	1.00 29.26
		ATOM	1906	C	GLU A 245	27.360	30.354	52.092	1.00 35.18
		ATOM	1907	0	GLU A 245	26.849	29.276	51.800	1.00 36.21
	20	MOTA	1908	CB	GLU A 245	26.908	32.177	50.421	1.00 30.22
	20	ATOM	1909	CG	GLU A 245	25.701	32.938	49.842	1.00 39.79
20		ATOM	1910	CD OF1	GLU A 245	26.026	33.564	48.529	1.00 51.91
		ATOM ATOM	1911 1912	OE1	GLU A 245 GLU A 245	26.945	34.351	48.358	1.00 34.19
		ATOM	1913	N N		25.246	33.142	47.585	1.00 47.48
	25	ATOM	1914	CA	ASP A 246 ASP A 246	28.570 29.417	30.484	52.680	1.00 32.29
	23	ATOM	1915	C	ASP A 246	28.848	29.350	53.033	1.00 30.70
		ATOM	1916	0	ASP A 246	28.881	28.645 27.417	54.230	1.00 35.47
		ATOM	1917	СВ	ASP A 246	30.873		54.347	1.00 37.08
25		ATOM	1918	CG	ASP A 246	31.709	29.717 28.473	53.355 53.413	1.00 33.17
	30	ATOM	1919		ASP A 246	31.934	27.789	52.437	1.00 64.49 1.00 67.15
		ATOM	1920		ASP A 246	32.118	28.167	54.622	1.00 79.01
		ATOM	1921	N	LEU A 247	28.323	29.434	55.134	1.00 33.59
		ATOM	1922	CA	LEU A 247	27.731	28.868	56.334	1.00 36.70
		ATOM	1923	С	LEU A 247	26.355	28.208	56.083	1.00 35.92
30	35	ATOM	1924	0	LEU A 247	26.060	27.110	56.551	1.00 30.77
		MOTA	1925	СВ	LEU A 247	27.562	29.954	57.435	1.00 38.34
		MOTA	1926	CG	LEU A 247	28.732	30.100	58.394	1.00 44.30
		ATOM	1927	CD1	LEU A 247	29.341	28.738	58.641	1.00 48.20
		MOTA	1928	CD2	LEU A 247	29.779	31.013	57.815	1.00 35.25
	40	MOTA	1929	N	GLY A 248	25.471	28.887	55.353	1.00 34.97
		MOTA	1930	CA	GLY A 248	24.160	28.315	55.181	1.00 36.00
35		ATOM	1931	С	GLY A 248	23.754	27.976	53.778	1.00 37.99
		MOTA	1932	0	GLY A 248	22.637	27.524	53.526	1.00 38.13
	4.5	ATOM	1933	N	GLY A 249	24.637	28.158	52.849	1.00 30.74
	45	ATOM	1934	CA	GLY A 249	24.203	27.852	51.526	1.00 30.15
		MOTA	1935	C	GLY A 249	23.918	29.131	50.759	1.00 38.91
		ATOM	1936	0	GLY A 249	24.126	30.240	51.238	1.00 41.32
40		ATOM	1937	N	PRO A 250	23.453	28.946	49.547	1.00 38.93
	50	ATOM	1938	CA	PRO A 250	23.173	30.021	48.639	1.00 38.03
	50	ATOM	1939	C	PRO A 250	22.203	31.078	49.096	1.00 42.17
		MOTA	1940	0	PRO A 250	21.258	30.823	49.840	1.00 45.20
		ATOM	1941	CB	PRO A 250	22.663	29.357	47.352	1.00 39.18
		MOTA MOTA	1942 1943	CG	PRO A 250 PRO A 250	22.952	27.864	47.436	1.00 41.01
	55	ATOM	1944			23.396	27.610	48.865	1.00 38.57
45	55	MOTA	1944	N CA	TYR A 251 TYR A 251	22.486 21.692	32.275	48.600	1.00 35.37
		MOTA	1946	C			33.461	48.817	1.00 34.87
		ATOM	1947	Ö	TYR A 251 TYR A 251	20.740 21.125	33.479	47.649	1.00 39.55
		ATOM	1947	СВ	TYR A 251	22.540	33.794	46.535	1.00 42.57
	60	ATOM	1949	CG	TYR A 251	21.711	34.759	48.790	1.00 35.07
	00	ATOM	1950		TYR A 251	21.711	35.980	49.119	1.00 35.25
50		MOTA	1951		TYR A 251	21.260	36.229 36.846	50.441 48.121	1.00 33.14 1.00 37.98
50		MOTA	1952		TYR A 251	20.575	37.341	50.781	1.00 37.98
		ATOM	1953		TYR A 251	20.492	37.967	48.443	1.00 20.05
							37.307	10.113	40.03

5		ATOM	1954	CZ	TYR	Α	251	20.160	38.213	49.777	1.00 42.84
		ATOM	1955	OH	TYR	Α	251	19.409	39.307	50.112	1.00 39.70
		ATOM	1956	N	VAL			19.510	33.102	47.914	1.00 32.21
		ATOM	1957	CA	VAL			18.495	33.003	46.899	1.00 30.05
	5	ATOM	1958	С	VAL			17.708	34.279	46.631	1.00 38.47
	-	ATOM	1959	ō	VAL			17.000	34.340	45.640	1.00 40.65
		ATOM	1960	СВ	VAL			17.560	31.845	47.253	1.00 31.27
10		ATOM	1961		VAL			18.378	30.605	47.643	1.00 28.15
		ATOM	1962		VAL			16.614	32.234	48.405	1.00 30.93
	10	ATOM	1963	N	TRP			17.800	35.292	47.504	1.00 32.44
	10	ATOM	1964	CA	TRP			17.041	36.509	47.309	1.00 30.93
		MOTA	1965	c	TRP			17.468	37.341	46.119	1.00 43.56
		ATOM	1966	Ö	TRP			16.690	38,119	45.568	1.00 45.70
		ATOM	1967	СВ	TRP			16.898	37.302	48.606	
15	15	ATOM	1968	CG	TRP			16.364	36.369	49.625	1.00 29.65
	10	ATOM	1969		TRP			17.086	35.546		1.00 30.19
		ATOM	1970		TRP					50.413	1.00 32.81
			1971					14.989	36.110	49.913	1.00 29.63
		ATOM			TRP			16.251	34.794	51.194	1.00 30.69
	20	MOTA	1972		TRP			14.955	35.128	50.912	1.00 31.50
	20	MOTA	1973		TRP			13.789	36.637	49.450	1.00 30.18
20		MOTA	1974		TRP			13.746	34.657	51.433	1.00 30.31
		MOTA	1975		TRP			12.600	36.164	49.958	1.00 31.14
		ATOM	1976		TRP			12.579	35.176	50.946	1.00 31.37
	26	ATOM	1977	N	GLY			18.697	37.182	45.675	1.00 42.35
	25	MOTA	1978	CA	GLY			19.101	37.944	44.509	1.00 41.34
		MOTA	1979	С	GLY			19.875	39.192	44.858	1.00 45.47
		ATOM	1980	0	GLY			21.079	39.236	44.671	1.00 45.89
25		MOTA	1981	N	GLN	A	255	19.160	40.210	45.351	1.00 41.86
		ATOM	1982	CA	GLN	Α	255	19.746	41.488	45.675	1.00 38.67
	30	MOTA	1983	С	GLN	A	255	19.576	41.776	47.153	1.00 40.18
		MOTA	1984	0	GLN	Α	255	18.494	41.811	47.659	1.00 38.67
		ATOM	1985	CB	GLN	Α	255	19.023	42.552	44.836	1.00 37.82
		ATOM	1986	CG	GLN	A	255	19.455	43.979	45.169	1.00 50.17
		ATOM	1987	CD	GLN			20.618	44.368	44.283	1.00 62.88
30	35	ATOM	1988	OE1	GLN			21.104	43.612	43.463	1.00 55.76
		ATOM	1989		GLN			21.057	45.625	44.479	1.00 34.97
		ATOM	1990	N	TYR			20.716	41.900	47.866	1.00 33.01
		ATOM	1991	CA	TYR			20.651	42.361	49.258	1.00 28.69
		ATOM	1992	C	TYR			20.891	43.854	49.329	1.00 26.72
	40	ATOM	1993	Ō	TYR			21.963	44.321	49.225	1.00 24.22
		ATOM	1994	СВ	TYR			21.743	41.629	50.075	1.00 29.99
35		MOTA	1995	CG	TYR			21.567	41.867	51.556	1.00 35.47
		ATOM	1996		TYR			20.582	41.200	52.250	1.00 35.76
		ATOM	1997		TYR			22.405	42.746	52.239	1.00 37.52
	45	ATOM	1998		TYR			20.436	41.396	53.599	
		ATOM	1999		TYR			22.255	42.946		1.00 25.80
		ATOM	2000	CZ	TYR			21.283	42.275	53.588	1.00 39.10
		ATOM	2001	OH	TYR					54.268	1.00 31.78
40		ATOM	2002					21.153	42.433	55.631	1.00 37.35
	50			N	ASP			19.834	44.613	49.463	1.00 23.26
	50	ATOM	2003	CA	ASP			20.077	46.027	49.621	1.00 23.47
		ATOM	2004	С	ASP			19.977	46.444	51.071	1.00 35.90
		ATOM	2005	0	ASP			19.729	45.661	51.967	1.00 39.48
		ATOM	2006	СВ	ASP			19.073	46.803	48.758	1.00 24.13
		MOTA	2007	CG	ASP	Α	257	19.689	47.030	47.388	1.00 38.50
45	55	ATOM	2008	OD1	ASP	Α	257	20.843	46.675	47.220	1.00 42.61
		ATOM	2009	OD2	ASP			19.020	47.555	46.517	1.00 29.02
		MOTA	2010	N	LEU	Α	258	20.370	47.661	51.386	1.00 30.86
		ATOM	2011	CA	LEU	Α	258	20.306	48.159	52.735	1.00 27.50
		ATOM	2012	С	LEU			19.526	49.466	52.765	1.00 36.37
	60	ATOM	2013	0	LEU			19.620	50.302	51.840	1.00 37.98
		ATOM	2014	СВ	LEU			21.727	48.442	53.274	1.00 24.71
50		ATOM	2015	CG	LEU			22.552	47.191	53.491	1.00 31.13
		MOTA	2016		LEU			23.913	47.567	54.043	
		ATOM	2017		LEU			21.854	46.282		1.00 30.89
		711 011	2017	CDZ	ne0	л	230	21.034	40.202	54.500	1.00 33.65

5		ATOM	2018	N	LEU A 259	18.762	49.632	53.838	1.00 29.87
		ATOM	2019	CA	LEU A 259		50.849	54.052	1.00 28.43
		ATOM	2020	С	LEU A 259		51.453	55.446	1.00 31.30
		ATOM	2021	ō	LEU A 259		50.819	56.477	1.00 31.19
	5	ATOM	2022	СВ	LEU A 259		50.809	53.693	1.00 27.63
	•	ATOM	2023	CG	LEU A 259		51.980	54.298	1.00 31.51
		ATOM	2024		LEU A 259		53.300	53.605	1.00 32.32
10		ATOM	2025		LEU A 259		51.731	54.253	1.00 26.87
		ATOM	2026	N	VAL A 260		52.683	55.447	1.00 25.88
	10	ATOM	2027	CA	VAL A 260		53.435	56.638	1.00 25.99
	10	ATOM	2028	c	VAL A 260		54.336	56.796	
		ATOM	2029	ŏ	VAL A 260				1.00 34.83
		ATOM	2030	CB	VAL A 260		55.187 54.234	55.959	1.00 41.92
		ATOM	2031		VAL A 260			56.408	1.00 29.97
15	15	ATOM	2032		VAL A 260		55.179	57.592	1.00 32.08
	13		2032		LEU A 261		53.295	56.130	1.00 26.15
		ATOM		N			54.120	57.815	1.00 28.41
		ATOM	2034	CA.	LEU A 261		54.878	58.024	1.00 25.52
		ATOM	2035	C	LEU A 261		56.054	58.948	1.00 29.42
	20	ATOM	2036	0	LEU A 261		56.300	59.489	1.00 29.96
	20	ATOM	2037	СВ	LEU A 261		53.921	58.706	1.00 25.70
20		ATOM	2038	CG	LEU A 261		52.877	57.740	1.00 33.14
		ATOM	2039		LEU A 261		51.571	57.929	1.00 32.73
		ATOM	2040		LEU A 261		52.686	57.935	1.00 43.74
	0.5	ATOM	2041	N	PRO A 262		56.758	59.142	1.00 28.52
	25	ATOM	2042	CA	PRO A 262		57.870	60.047	1.00 28.50
		MOTA	2043	C	PRO A 262	15.152	57.294	61.432	1.00 35.36
		ATOM	2044	0	PRO A 262	14.866	56.124	61.683	1.00 34.52
25		ATOM	2045	CB	PRO A 262	13.512	58.512	59.971	1.00 29.19
		ATOM	2046	CG	PRO A 262	12.707	57.719	58.964	1.00 34.34
	30	ATOM	2047	CD	PRO A 262	13.581	56.575	58.492	1.00 30.63
		ATOM	2048	N	PRO A 263	15.706	58.105	62.327	1.00 31.50
		ATOM	2049	CA	PRO A 263	16.060	57.657	63.673	1.00 28.77
		ATOM	2050	С	PRO A 263	14.966	57.021	64.493	1.00 29.15
		ATOM	2051	0	PRO A 263		56.335	65.434	1.00 26.36
30	35	ATOM	2052	СВ	PRO A 263		58.867	64.392	1.00 29.16
		ATOM	2053	CG	PRO A 263		59.954	63.335	1.00 31.55
		ATOM	2054	CD	PRO A 263		59.558	62.138	1.00 29.17
		ATOM	2055	N	SER A 264	13.712	57.258	64.143	1.00 33.87
		ATOM	2056	CA	SER A 264		56.703	64.864	1.00 33.81
	40	ATOM	2057	С	SER A 264		55.223	64.604	1.00 37.36
		ATOM	2058	0	SER A 264		54.570	65.201	1.00 39.61
35		ATOM	2059	СВ	SER A 264	11.280	57.423	64.576	1.00 35.61
		ATOM	2060	OG	SER A 264	10.955	57.276	63.201	1.00 53.45
		ATOM	2061	N	PHE A 265		54.684	63.710	1.00 29.00
	45	ATOM	2062	CA	PHE A 265		53.256	63.453	1.00 28.56
		ATOM	2063	C	PHE A 265		52.491	64.787	1.00 28.49
		ATOM	2064	ō	PHE A 265		52.675	65.533	1.00 27.36
40		ATOM	2065	СВ	PHE A 265		52.833	62.454	1.00 27.30
40		ATOM	2066	CG	PHE A 265		51.458	62.028	
	50	ATOM	2067		PHE A 265		51.174	61.543	1.00 34.51
	50	ATOM	2068		PHE A 265		50.435	62.156	1.00 35.11
		ATOM	2069		PHE A 265				
		ATOM	2070				49.876	61.154	1.00 37.42
					PHE A 265		49.131	61.772	1.00 42.65
45	55	ATOM	2071	CZ	PHE A 265		48.860	61.274	1.00 40.14
45	22	ATOM	2072	N	PRO A 266		51.650	65.128	1.00 24.06
		ATOM	2073	CA	PRO A 266		50.945	66.419	1.00 20.62
		ATOM	2074	C	PRO A 266		49.794	66.701	1.00 29.34
		MOTA	2075	0	PRO A 266		49.364	67.847	1.00 28.17
	C O	MOTA	2076	CB	PRO A 266		50.463	66.593	1.00 19.16
	60	ATOM	2077	CG	PRO A 266		50.686	65.281	1.00 21.07
50		MOTA	2078	CD	PRO A 266		51.355	64.325	1.00 19.44
50		MOTA	2079	N	TYR A 267		49.280	65.676	1.00 27.23
		ATOM	2080	CA	TYR A 267		48.160	65.817	1.00 25.74
		ATOM	2081	С	TYR A 267	16.181	48.454	65.189	1.00 32.57

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5		ATOM	2082	0	TYR	A	267	16.2	81	49.316	64.324	1.00 32.48
		ATOM	2083	СВ	TYR			14.2		46.903	65.121	1.00 25.07
		ATOM	2084	CG	TYR	Α	267	12.9		46.502	65.674	1.00 24.45
		ATOM	2085	CD1	TYR	Α	267	12.9	15	45.765	66.856	1.00 27.05
	5	ATOM	2086	CD2	TYR	А	267	11.7	76	46.851	65.037	1.00 22.15
		ATOM	2087	CE1	TYR	Α	267	11.6	97	45.387	67.419	1.00 25.01
10		ATOM	2088	CE2	TYR	A	267	10.5	48	46.496	65.596	1.00 19.09
		ATOM	2089	CZ	TYR	Α	267	10.5	10	45.767	66.786	1.00 17.98
		ATOM	2090	OH	TYR	Α	267	9.3	02	45.416	67.353	1.00 19.51
	10	ATOM	2091	N	GLY	Α	268	17.1	96	47.698	65.627	1.00 30.22
		ATOM	2092	CA	GLY	А	268	18.5	47	47.826	65.114	1.00 27.29
		ATOM	2093	С	GLY	Α	268	18.4	85	47.620	63.614	1.00 29.82
		ATOM	2094	0	GLY	Α	268	19.1	36	48.297	62.836	1.00 32.99
15		ATOM	2095	N	GLY	Α	269	17.6	37	46.676	63.228	1.00 23.19
	15	ATOM	2096	CA	GLY			17.3		46.320	61.853	1.00 21.62
		MOTA	2097	С	GLY			16.1		45.402	61.777	1.00 27.53
		ATOM.	2098	0	GLY			15.6		44.948	62.820	1.00 20.14
		ATOM	2099	N	MET			15.7		45.154	60.528	1.00 27.81
		ATOM	2100	CA	MET			14.6		44.267	60.176	1.00 25.61
	20	ATOM	2101	С	MET			14.9		43.585	58.874	1.00 33.56
20		ATOM	2102	0	MET			15.2		44.247	57.867	1.00 34.67
		ATOM	2103	СВ	MET			13.2		44.936	60.028	1.00 26.07
		MOTA	2104	CG	MET			12.1		43.937	59.602	1.00 28.81
	25	ATOM	2105	SD	MET			11.8		42.742	60.929	1.00 37.39
	25	ATOM	2106	CE	MET			10.7		41.621	60.082	1.00 35.30
		ATOM	2107	N	GLU			14.9		42.263	58.904	1.00 32.20
25		ATOM	2108	CA	GLU			15.3		41.459	57.753	1.00 33.32
25		ATOM	2109	С	GLU			14.4		41.382	56.567	1.00 40.86
	20	ATOM	2110	0	GLU			14.0		40.285	56.107	1.00 42.02
	30	ATOM	2111	CB	GLU			15.8		40.054	58.230	1.00 35.05
		ATOM	2112	CG	GLU			14.6		39.218	58.760	1.00 33.55
		ATOM	2113	CD	GLU			14.2		39.428	60.219	1.00 25.52
		ATOM	2114		GLU			14.5		40.436	60.844	1.00 37.23
30	35	ATOM	2115		GLU			13.6		38.393	60.757	1.00 25.86
	33	ATOM	2116	N	ASN			13.9		42.535	56.052	1.00 35.34
		ATOM	2117 2118	CA C	ASN			13.0		42.544	54.928	1.00 33.26
		ATOM ATOM	2119	0	ASN ASN			13.7 14.8		42.048	53.702	1.00 34.47
		ATOM	2120	СВ	ASN			12.4		42.613 43.947	53.351	1.00 33.64
	40	ATOM	2121	CG	ASN			11.6		44.453	54.719 55.935	1.00 30.65
05	40	ATOM	2122		ASN			11.9		45.554	56.475	1.00 42.50 1.00 47.09
35		ATOM	2123		ASN			10.7		43.661	56.371	1.00 24.31
		ATOM	2124	N	PRO			13.2		40.983	53.078	1.00 29.63
		ATOM	2125	CA	PRO			13.9		40.373	51.910	1.00 28.47
	45	ATOM	2126	c	PRO			14.3		41.345	50.819	1.00 30.43
		ATOM	2127	ŏ	PRO			13.4		42.089	50.372	1.00 30.45
		ATOM	2128	СВ	PRO			12.9		39.305	51.381	1.00 30.16
40		ATOM	2129	CG	PRO			11.8		39.237	52.365	1.00 36.65
		ATOM	2130	CD	PRO			11.9		40.440	53.310	1.00 30.84
	50	MOTA	2131	N	CYS			15.5		41.333	50.431	1.00 27.40
		MOTA	2132	CA	CYS			16.0		42.206		1.00 28.17
		ATOM	2133	С	CYS			16.3		43.604	49.860	1.00 27.35
		MOTA	2134	0			274	17.1		44.345	49.248	1.00 28.53
		ATOM	2135	CB	CYS	Α	274	15.1	.21	42.347	48.145	1.00 32.00
45	55	ATOM	2136	SG	CYS	Α	274	14.6	559	40.798	47.340	1.00 38.42
		MOTA	2137	N	LEU	Α	275	15.6	558	43.972	50.947	1.00 26.20
		ATOM	2138	CA	LEU			15.7	89	45.315	51.535	1.00 29.54
		ATOM	2139	С	LEU			15.8		45.279	53.059	1.00 32.52
		ATOM	2140	0	LEU			14.8		45.250	53.772	1.00 32.44
	60	MOTA	2141	СВ			275	14.6		46.253	51.005	1.00 28.58
50		MOTA	2142	CG	LEU			14.8	347	47.735	51.239	1.00 26.78
50		MOTA	2143	CD1	LEU	Α	275	16.1	.91	48.183	50.698	1.00 21.90
		ATOM	2144	CD2	LEU			13.7		48.478	50.554	1.00 31.48
		ATOM	2145	N	THR	Α	276	17.0	62	45.244	53.570	1.00 29.67

5										
_		ATOM	2146	CA	THR A		17.225	45.198	54.996	1.00 30.47
		ATOM	2147	C	THR A		17.120	46.624	55.597	1.00 34.60
		ATOM	2148	0	THR A		17.766	47.588	55.129	1.00 31.01
	_	MOTA	2149	CB	THR A		18.508	44.397	55.387	1.00 30.98
	5	MOTA	2150	OG1			18.224	43.030	55.512	1.00 42.01
		MOTA	2151		THR A		19.124	44.835	56.694	1.00 29.43
10		ATOM	2152	N	PHE A		16.280	46.759	56.622	1.00 27.69
		MOTA	2153	CA	PHE A		16.164	48.034	57.274	1.00 28.92
	10	ATOM	2154	C	PHE A		17.184	48.065	58.403	1.00 36.07
	10	ATOM	2155 2156	O CB	PHE A		17.337	47.088	59.131	1.00 34.57
		ATOM ATOM	2157	CG	PHE A		14.791 13.774	48.265	57.901 56.848	1.00 30.17
		ATOM	2158		PHE A		14.011	48.458 47.966		1.00 30.72
15		ATOM	2159		PHE A		12.573	49.114	55.568 57.105	1.00 30.73
15	15	ATOM	2160		PHE A		13.072	48.135	54.552	1.00 29.30
	1.5	ATOM	2161		PHE A		11.619	49.276	56.101	1.00 32.26
		ATOM	2162	CZ	PHE A		11.862	48.772	54.824	1.00 32.20
		ATOM	2163	N	VAL A		17.864	49.186	58.562	1.00 32.97
		ATOM	2164	CA	VAL A		18.839	49.338	59.614	1.00 32.66
	20	ATOM	2165	c	VAL A		18.696	50.698	60.248	1.00 37.01
20		ATOM	2166	ŏ	VAL A		18.251	51.635	59.599	1.00 37.16
		ATOM	2167	СВ	VAL A		20,246	49.088	59.109	1.00 36.51
		ATOM	2168		VAL A		20.173	47.967	58.086	1.00 37.40
		ATOM	2169		VAL A		20.791	50.356	58.444	1.00 34.87
	25	ATOM	2170	N	THR A		19.066	50.778	61.515	1.00 32.36
		ATOM	2171	CA	THR A		18.948	51.994	62.264	1.00 31.03
2		ATOM	2172	С	THR A	279	20.121	52.883	62.035	1.00 37.42
25		ATOM	2173	0	THR A	279	21.243	52.397	61.920	1.00 39.87
		ATOM	2174	CB	THR A	279	18.885	51.695	63.759	1.00 31.39
	30	ATOM	2175	OG1	THR A	279	19.110	52.895	64.472	1.00 34.21
		ATOM	2176	CG2	THR A	279	19.989	50.706	64.083	1.00 23.69
		ATOM	2177	N	PRO A	280	19.845	54.187	62.000	1.00 30.07
		MOTA	2178	CA	PRO A		20.903	55.132	61.802	1.00 27.00
30	25	ATOM	2179	С	PRO A		21.823	55.110	63.005	1.00 30.60
	35	ATOM	2180	0	PRO A		22.951	55.588	62.934	1.00 30.20
		ATOM	2181	СВ	PRO A		20.249	56.497	61.601	1.00 26.23
		MOTA	2182	CG	PRO A		18.769	56.337	61.889	1.00 28.07
		ATOM	2183	CD	PRO A		18.499	54.848	61.984	1.00 26.11
	40	ATOM	2184	N	THR A		21.348	54.509	64.112	1.00 27.82
	40	ATOM	2185	CA	THR A		22.199	54.426	65.302	1.00 27.48
35		ATOM ATOM	2186 2187	C	THR A		23.372	53.523	65.073	1.00 31.37
		ATOM	2188	O CB	THR A		24.226 21.499	53.385 54.016	65.944 66.601	1.00 31.93
		ATOM	2189	OG1			21.021	52.681	66.524	1.00 21.45 1.00 33.18
	45	ATOM	2190	CG2	THR A		20.388	54.994	66.874	1.00 33.18
		ATOM	2191	N	LEU A		23.378	52.881	63.913	1.00 25.29
		MOTA	2192	CA	LEU A		24.473	51.993	63.586	1.00 24.04
40		ATOM	2193	C	LEU A		25.682	52.790	63.049	1.00 34.74
		ATOM	2194	ŏ	LEU A		26.787	52.279	62.884	1.00 34.84
	50	ATOM	2195	CB	LEU A		24.063	51.038	62.464	1.00 22.14
		ATOM	2196	CG	LEU A		23.104	49.916	62.819	1.00 26.88
		MOTA	2197		LEU A		23.312	48.809	61.791	1.00 27.77
		ATOM	2198		LEU A		23.322	49.404	64.249	1.00 21.75
		ATOM	2199	N	LEU A	283	25.465	54.063	62.744	1.00 32.05
45	55	MOTA	2200	CA	LEU A	283	26.501	54.903	62.159	1.00 31.43
		ATOM	2201	С	LEU A		27.659	55.324	63.055	1.00 41.94
		MOTA	2202	0	LEU A	283	27.907	56.525	63.196	1.00 49.19
		MOTA	2203	CB	LEU A		25.861	56.117	61.418	1.00 29.55
		MOTA	2204	CG	LEU A		24.720	55.661	60.488	1.00 32.94
	60	MOTA	2205		LEU A		23.933	56.811	59.869	1.00 33.48
50		MOTA	2206		LEU A		25.232	54.716	59.409	1.00 28.39
		ATOM	2207	N	ALA A		28.387	54.370	63.638	1.00 33.18
		ATOM	2208	CA	ALA A		29.488	54.728	64.532	1.00 30.20
		ATOM	2209	С	ALA A	284	30.655	55.492	63.922	1.00 31.97

5		ATOM	2210	0	ALA A 284	31.411	56.165	64.642	1.00 31.40
		ATOM	2211	СВ	ALA A 284	29.973	53.544	65.336	1.00 29.60
		ATOM	2212	N	GLY A 285	30.801	55.371	62.605	1.00 27.10
		ATOM	2213	CA	GLY A 285	31.882	56.018	61.867	1.00 29.77
	5	ATOM	2214	c	GLY A 285	33.174	55.194	61.910	1.00 39.25
	,	ATOM	2215	õ	GLY A 285	34.264	55.649	61.544	1.00 33.23
		ATOM	2216	N	ASP A 286	33.022	53.951	62.363	1.00 34.57
10		ATOM	2217	CA	ASP A 286	34.144	53.957	62.473	1.00 34.57
					ASP A 286	33.805	51.625		
	10	MOTA	2218	C				62.130	1.00 31.59
	10	ATOM	2219	0	ASP A 286	34.609 34.812	50.743	62.325	1.00 29.27
		ATOM	2220	CB	ASP A 286		53.163	63.860	1.00 34.65
		ATOM	2221	CG	ASP A 286	34.081	52.447	64.945	1.00 41.93
		ATOM	2222		ASP A 286	33.008	51.893	64.765	1.00 45.21
15	1.5	ATOM	2223		ASP A 286	34.714	52.492	66.087	1.00 35.67
	15	ATOM	2224	N	LYS A 287	32.590	51.395	61.641	1.00 29.46
		ATOM	2225	CA	LYS A 287	32.199	50.038	61.272	1.00 31.62
		ATOM	2226	С	LYS A 287	31.976	49.060	62.437	1.00 37.91
		ATOM	2227	0	LYS A 287	31.761	47.879	62.240	1.00 37.91
		ATOM	2228	CB	LYS A 287	33.215	49.447	60.304	1.00 32.17
	20	ATOM	2229	CG	LYS A 287	33.510	50.358	59.119	1.00 51.60
20		ATOM	2230	CD	LYS A 287	33.960	49.601	57 .87 7	1.00 50.74
		ATOM	2231	CE	LYS A 287	35.290	50.105	57.328	1.00 63.80
		ATOM	2232	NZ	LYS A 287	35.167	50.866	56.069	1.00 71.91
		ATOM	2233	N	SER A 288	32.168	49.575	63.647	1.00 31.58
	25	ATOM	2234	CA	SER A 288	32.079	48.737	64.810	1.00 27.15
		ATOM	2235	С	SER A 288	30.742	48.137	65.142	1.00 36.08
		ATOM	2236	ō	SER A 288	30.676	47.318	66.057	1.00 37.87
25		ATOM	2237	СВ	SER A 288	32.618	49.463	66.005	1.00 16.31
		ATOM	2238	OG	SER A 288	31.659	50.443	66.312	1.00 10.31
	30	ATOM	2239		LEU A 289		48.529		
	30			N		29.669		64.460	1.00 29.34
		ATOM	2240	CA	LEU A 289	28.351	47.979	64.794	1.00 24.70
		ATOM	2241	C	LEU A 289	27.792	47.105	63.686	1.00 32.97
		ATOM	2242	0	LEU A 289	26.591	46.766	63.648	1.00 30.35
30	25	ATOM	2243	CB	LEU A 289	27.385	49.090	65.191	1.00 21.45
	35	MOTA	2244	CG	LEU A 289	27.954	49.887	66.347	1.00 22.99
		ATOM	2245		LEU A 289	26.881	50.769	66.950	1.00 20.66
		ATOM	2246		LEU A 289	28.381	48.881	67.394	1.00 29.65
		ATOM	2247	N	SER A 290	28.723	46.753	62.801	1.00 31.21
	4.0	ATOM	2248	CA	SER A 290	28.453	45.941	61.645	1.00 29.89
	40	ATOM	2249	С	SER A 290	27.861	44.582	62.006	1.00 30.57
35		ATOM	2250	0	SER A 290	27.299	43.872	61.153	1.00 29.73
		ATOM	2251	CB	SER A 290	29.704	45.800	60.783	1.00 29.27
		ATOM	2252	OG	SER A 290	30.470	44.725	61.266	1.00 38.77
		ATOM	2253	N	ASN A 291	27.980	44.207	63.282	1.00 26.55
	45	ATOM	2254	CA	ASN A 291	27.449	42.909	63.706	1.00 25.78
		ATOM	2255	С	ASN A 291	26.006	42.773	63.355	1.00 30.89
		ATOM	2256	Ō	ASN A 291	25.576	41.702	62.975	1.00 29.73
40		ATOM	2257	СВ	ASN A 291	27.725	42.503	65.157	1.00 28.48
		ATOM	2258	CG	ASN A 291	26.910	43.313	66.119	1.00 33.33
	50	ATOM	2259		ASN A 291	27.065	44.529	66.198	1.00 34.48
	-	ATOM	2260		ASN A 291			66.818	1.00 28.96
		ATOM	2261	N	VAL A 292		43.885	63.476	1.00 20.50
		ATOM	2262	CA	VAL A 292		43.924	63.142	1.00 30.00
45	55	ATOM ATOM	2263 2264	0	VAL A 292		43.619	61.669	1.00 32.61
,,,	33				VAL A 292		43.082	61.255	1.00 33.31
		ATOM	2265	CB	VAL A 292		45.289	63.505	1.00 35.13
		ATOM	2266		VAL A 292		45.486	62.946	1.00 33.48
		ATOM	2267		VAL A 292		45.478	65.014	1.00 35.02
		ATOM	2268	N	ILE A 293		43.975	60.861	1.00 27.92
	60	ATOM	2269	CA	ILE A 293		43.685	59.461	1.00 28.71
50		ATOM	2270	С	ILE A 293		42.159	59.296	1.00 35.03
50		ATOM	2271	0	ILE A 293	23.860	41.475	58.624	1.00 38.34
		ATOM	2272	CB	ILE A 293	25.554	44.438	58.606	1.00 33.84
		ATOM	2273	CG1	ILE A 293	25.608	45.952	58.898	1.00 34.55

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5		ATOM	2274	CG2	ILE A 2	293	25.305	44.186	57.121	1.00 36.50
		MOTA	2275	CD1	ILE A 2	293	24.265	46.680	58.808	1.00 30.49
		ATOM	2276	N	ALA A 2	294	25.668	41.584	59.934	1.00 23.76
		ATOM	2277	CA	ALA A	294	25.836	40.138	59.809	1.00 19.95
	5	MOTA	2278	С	ALA A 2	294	24.559	39.409	60.165	1.00 27.33
		MOTA	2279	0	ALA A 2	294	24.183	38.422	59.505	1.00 25.48
10		MOTA	2280	CB	ALA A		26.984	39.644	60.688	1.00 19.24
		ATOM	2281	N	HIS A	295	23.917	39.934	61.244	1.00 27.63
		ATOM	2282	CA	HIS A		22.666	39.414	61.797	1.00 26.83
	10	ATOM	2283	С	HIS A		21.611	39.383	60.734	1.00 28.61
		MOTA	2284	0	HIS A		21.169	38.301	60.348	1.00 25.72
		MOTA	2285	СВ	HIS A		22.148	40.175	63.028	1.00 27.98
.2		MOTA	2286	CG	HIS A		20.937	39.534	63.657	1.00 31.62
15	1.5	ATOM	2287		HIS A		21.047	38.675	64.763	1.00 32.66
	15	ATOM	2288		HIS A		19.602	39.643	63.338	1.00 30.92
		ATOM	2289		HIS A		19.802	38.298	65.088	1.00 30.14
		MOTA	2290		HIS A		18.916	38.860	64.254	1.00 30.24
		ATOM	2291	N	GLU A		21.257	40.590	60.251	1.00 27.23
	20	ATOM	2292	CA	GLU A		20.266	40.749	59.195	1.00 25.98
20	20	ATOM ATOM	2293 2294	С 0	GLU A		19.628	39.790 39.081	58.056 57.561	1.00 32.73
20		ATOM	2295	СВ	GLU A		20.046	42.203	58.728	1.00 31.88
		ATOM	2296	CG	GLU A		19.892	43.148	59.936	1.00 24.55 1.00 23.16
		ATOM	2297	CD	GLU A		18.939	42.632	60.991	1.00 23.10
	25	ATOM	2298		GLU A		17.964	41.956	60.700	1.00 23.99
	20	ATOM	2299		GLU A		19.237	43.006	62.233	1.00 32.77
		ATOM	2300	N	ILE A		21.803	39.745	57.675	1.00 25.37
25		ATOM	2301	CA	ILE A		22.195	38.870	56.599	1.00 22.64
		ATOM	2302	c c	ILE A		21.812	37.445	56.859	1.00 27.47
	30	MOTA	2303	ō	ILE A		21.175	36.799	56.048	1.00 26.25
		ATOM	2304	СВ	ILE A		23.672	38.963	56.302	1.00 24.19
		ATOM	2305		ILE A		23.920	40.140	55.355	1.00 25.28
		ATOM	2306		ILE A		24.079	37.686	55.626	1.00 20.77
30		ATOM	2307	CD1	ILE A	297	25.325	40.705	55.435	1.00 16.26
30	35	MOTA	2308	N	SER A	298	22.226	36.947	58.012	1.00 28.23
		MOTA	2309	CA	SER A	298	21.939	35.569	58.377	1.00 25.04
		MOTA	2310	C ·	SER A		20.467	35.235	58.298	1.00 26.21
		MOTA	2311	0	SER A		20.118	34.097	58.000	1.00 26.30
	40	ATOM	2312	CB	SER A		22.520	35.209	59.714	1.00 27.82
	40	ATOM	2313	OG	SER A		23.890	35.552	59.714	1.00 35.98
35		MOTA	2314	N	HIS A		19.599	36.230	58.562	1.00 22.17
		ATOM	2315	CA	HIS A		18.205	36.092	58.719	1.00 22.77
		ATOM	2316	C	HIS A		17.614	35.710	57.387	1.00 29.10
	45	ATOM	2317 2318	0	HIS A		16.553	35.162 37.432	57.290	1.00 31.50
	43	ATOM ATOM	2319	CB CG	HIS A		17.662 17.053	37.432	59.200 60.602	1.00 24.67 1.00 29.10
		ATOM	2320		HIS A		16.190	36.368	60.975	1.00 29.10
40		ATOM	2321		HIS A		17.196	38.233	61.667	1.00 30.70
40		ATOM	2322		HIS A		15.811	36.675	62.233	1.00 32.33
	50	ATOM	2323		HIS A		16.397	37.783	62.674	1.00 31.74
	-	ATOM	2324	N	SER A		18.356	36.048	56.315	1.00 23.31
		ATOM	2325	CA	SER A		17.942	35.581	55.010	1.00 24.24
		ATOM	2326	c	SER A		17.879	34.050	54.977	1.00 34.13
		ATOM	2327	0	SER A		17.075	33.463	54.305	1.00 33.28
45	55	MOTA	2328	СВ	SER A		18.941	36.092	53.965	1.00 27.31
		MOTA	2329	OG	SER A	300	18.947	37.519	53.962	1.00 49.96
		ATOM	2330	N	TRP A		18.773	33.411	55.752	1.00 33.09
		ATOM	2331	CA	TRP A		18.702	31.969	55.829	1.00 31.84
		ATOM	2332	С	TRP A		17.740	31.511	56.895	1.00 32.15
	60	ATOM	2333	0	TRP A		16.764	30.876	56.620	1.00 27.05
50		ATOM	2334	CB	TRP A	301	20.095	31.429	56.082	1.00 30.16
		ATOM	2335	CG	TRP A		20.791	31.421	54.801	1.00 32.02
		ATOM	2336		TRP A		20.787	30.393	53.859	1.00 35.05
		ATOM	2337	CD2	TRP A	301	21.496	32.520	54.202	1.00 30.84

5		MOTA	2338	NE1	TRP A	301	21.415	30.732	52.722	1.00 33.29
		ATOM	2339	CE2	TRP A	301	21.886	32.112	52.921	1.00 33.44
		MOTA	2340	CE3	TRP A	301	21.811	33.790	54.631	1.00 32.65
		MOTA	2341	CZ2	TRP A	301	22.577	32.970	52.108	1.00 32.21
	5	ATOM	2342	C23	TRP A	301	22.503	34.652	53.812	1.00 36.10
		MOTA	2343	CH2	TRP A	301	22.888	34.239	52.544	1.00 36.83
		MOTA	2344	N	THR A	302	18.042	31.864	58.146	1.00 31.77
10		ATOM	2345	CA	THR A		17.125	31.488	59.215	1.00 33.55
		ATOM	2346	C	THR A		16.276	32.690	59.695	1.00 36.35
	10	ATOM	2347	0	THR A		16.759	33.590	60.330	1.00 36.56
		MOTA	2348	CB	THR A		17.963	30.920	60.366	1.00 31.04
		ATOM	2349		THR A		19.047	31.807	60.639	1.00 38.50
		MOTA	2350		THR A		18.544	29.555	59.967	1.00 17.10
		MOTA	2351	N	GLY A		15.053	32.418	59.250	1.00 25.28
15	15	ATOM	2352	CA	GLY A		13.908	33.236	59.483	1.00 21.59
		ATOM	2353	С	GLY A		13.202	33.382	58.163	1.00 26.99
		ATOM	2354	ō	GLY A		12.040	33.040	57.994	1.00 26.18
		ATOM	2355	N	ASN A		13.936	33.891	57.195	1.00 28.05
		ATOM	2356	CA	ASN A		13.363	34.101	55.875	1.00 28.17
	20	ATOM	2357	C	ASN A		13.141	32.839	55.056	1.00 28.99
		ATOM	2358	ō	ASN A		12.118	32.715	54.415	1.00 24.87
20		ATOM	2359	СВ	ASN A		14.091	35.176	55.047	
		ATOM	2360	CG	ASN A		14.133	36.499	55.757	1.00 23.55 1.00 37.80
		ATOM	2361		ASN A		13.630	36.613		
	25	ATOM	2362		ASN A		14.752	37.488	56.892	1.00 20.66
		ATOM	2363	N	LEU A		14.110		55.093	1.00 24.17
		ATOM	2364	CA	LEU A			31.919	55.055	1.00 27.24
		ATOM	2365	C			13.987	30.677	54.306	1.00 27.34
25					LEU A		13.218	29.665	55.121	1.00 31.29
	30	ATOM	2366 2367	O			12.235	29.051	54.678	1.00 29.23
	30	ATOM		CB	LEU A		15.371	30.119	53.967	1.00 27.62
		ATOM	2368	CG	LEU A		15.805	30.593	52.603	1.00 32.23
		ATOM	2369		LEU A		17.289	30.293	52.412	1.00 28.91
		ATOM	2370		LEU A		14.951	29.887	51.549	1.00 41.51
	35	ATOM	2371	N	VAL A		13.711	29.528	56:347	1.00 27.75
30	33	ATOM	2372	CA	VAL A		13.134	28.652	57.327	1.00 29.99
		ATOM	2373	С	VAL A		12.578	29.527	58.403	1.00 31.78
		ATOM	2374	0	VAL A		13.306	30.217	59.110	1.00 28.32
		ATOM	2375	CB	VAL A		14.092	27.593	57.827	1.00 37.24
	40	ATOM	2376		VAL A		15.479	28.180	57.969	1.00 38.36
	40	ATOM	2377		VAL A		13.602	27.107	59.164	1.00 37.56
35		ATOM	2378	N	THR A		11.259	29.517	58.440	1.00 29.40
33		ATOM	2379	CA	THR A		10.499	30.358	59.320	1.00 28.14
		ATOM	2380	С	THR A		9.729	29.712	60.446	1.00 34.06
	45	ATOM	2381	0	THR A		9.029	28.706	60.277	1.00 36.72
	45	MOTA	2382	CB	THR A		9.474	31.115	58.460	1.00 23.03
		ATOM	2383		THR A		10.124	31.811	57.422	1.00 28.56
		ATOM	2384		THR A		8.665	32.068	59.336	1.00 12.55
40		ATOM	2385	N	ASN A		9.802	30.347	61.608	1.00 29.29
	50	ATOM	2386	CA	ASN A		9.042	29.862	62.724	1.00 27.82
	50	ATOM	2387	С	ASN A		7.576	29.716	62.234	1.00 31.42
		MOTA	2388	0	ASN A		7.072	30.535	61.450	1.00 32.96
		ATOM	2389	СВ	ASN A		9.194	30.790	63.972	1.00 23.57
		ATOM	2390	CG	ASN A		8.935	32.298	63.745	1.00 30.38
	~ ~	ATOM	2391		ASN A		9.505	33.190	64.400	1.00 23.70
45	55	MOTA	2392	ND2	ASN A	308	8.056	32.608	62.818	1.00 41.34
		ATOM	2393	N	LYS A	309	6.890	28.658	62.640	1.00 24.10
		ATOM	2394	CA	LYS A		5.502	28.433	62.230	1.00 23.40
		ATOM	2395	С	LYS A	309	4.514	29.380	62.964	1.00 28.17
		ATOM	2396	0	LYS A	309	3.430	29.756	62.474	1.00 22.88
	60	ATOM	2397	CB	LYS A		5.151	26.975	62.459	1.00 24.26
		ATOM	2398	CG	LYS A		4.036	26.478	61.555	1.00 28,57
50		ATOM	2399	ÇD	LYS A		3.543	25.075	61.924	1.00 38.25
		ATOM	2400	CE	LYS A		3.475	24.112	60.739	1.00 78.39
		ATOM	2401	NZ	LYS A		4.389	22.953	60.849	1.00 98.22
							,		55.545	

5		ATOM	2402	N	THR	Α	310	4.917	29.744	64.179	1.00 23.46
		ATOM	2403	CA	THR	Α	310	4.179	30.616	65.037	1.00 22.98
		ATOM	2404	C	THR	Α	310	5.142	31.336	65.922	1.00 31.43
		ATOM	2405	0	THR	Α	310	6.223	30.836	66.230	1.00 31.51
	5	ATOM	2406	CB	THR	Α	310	3.104	29.917	65.871	1.00 34.01
		ATOM	2407	OG1	THR	Α	310	3.684	29.148	66.945	1.00 27.97
		ATOM	2408	CG2	THR	Α	310	2.174	29.114	64.956	1.00 24.58
10		ATOM	2409	N	TRP			4.733	32.527	66.299	1.00 29.82
		ATOM	2410	CA	TRP			5.559	33.371	67.120	1.00 30.49
	10	ATOM	2411	С	TRP			6.044	32.692	68.381	1.00 26.99
		ATOM	2412	0	TRP			7.015	33.101	68.971	1.00 25.15
		ATOM	2413	CB	TRP			4.933	34.768	67.320	1.00 30.34
		ATOM	2414	CG	TRP	Α	311	4.706	35.412	66.001	1.00 30.63
		ATOM	2415	CD1	TRP	Α	311	3.514	35.785	65.490	1.00 32.07
15	15	ATOM	2416	CD2	TRP	Α	311	5.705	35.723	65.008	1.00 31.31
		ATOM	2417		TRP			3.703	36.335	64.250	1.00 29.97
		ATOM	2418		TRP			5.033	36.317	63.931	1.00 32.88
		ATOM	2419		TRP			7.099	35.586	64.943	1.00 31.44
		ATOM	2420		TRP			5.721	36.771	62.804	1.00 31.56
	20	ATOM	2421		TRP			7.779	36.059	63.848	1.00 30.39
20		ATOM	2422		TRP			7.089	36.639	62.789	1.00 30.58
20		ATOM	2423	N	ASP			5.366	31.632	68.770	1.00 27.36
		ATOM	2424	CA	ASP			5.757	30.868	69.950	1.00 27.38
		ATOM	2425	c	ASP			7.149	30.213	69.757	1.00 27.30
	25	ATOM	2426	ŏ	ASP			7.826	29.802	70.718	1.00 27.07
		ATOM	2427	СВ	ASP			4.697	29.750	70.713	1.00 25.96
		ATOM	2428	CG	ASP			3.432	30.230	70.217	1.00 23.98
25		ATOM	2429		ASP			3.197	31.396	71.102	1.00 27.42
25		ATOM	2430		ASP			2.623	29.265	71.208	1.00 29.33
	30	ATOM	2431	N	HIS			7.562	30.089	68.487	1.00 25.04
	50	ATOM	2432	CA	HIS			8.820	29.454	68.164	1.00 23.48
		ATOM	2433	c	HIS			9.864	30.452	67.737	
		ATOM	2434	ŏ	HIS			10.929	30.139	67.214	1.00 25.38
		ATOM	2435	СВ	HIS			8.588	28.245	67.209	1.00 29.97 1.00 25.00
30	35	ATOM	2436	CG	HIS			7.641	27.230	67.837	1.00 29.77
	55	ATOM	2437		HIS			8.087	26.183	68.635	
		ATOM	2438		HIS			6.279	27.152	67.808	1.00 31.37 1.00 31.31
		ATOM	2439		HIS			7.015	25.509		
		ATOM	2440		HIS			5.913	26.066	69.039 68.559	1.00 28.91 1.00 29.40
	40	ATOM	2441	N	PHE			9.521	31.682	68.005	
		ATOM	2442	CA	PHE			10.345	32.810	67.701	1.00 17.43
35		ATOM	2443	C	PHE			11.852	32.523	67.701	1.00 17.16
		ATOM	2444	ŏ	PHE			12.669	32.923	66.963	1.00 26.01
		ATOM	2445	СВ	PHE			9.908	34.056	68.517	1.00 30.40 1.00 18.63
	45	ATOM	2446	CG	PHE			10.592	35.351	68.113	
		ATOM	2447		PHE			10.712	35.697	66.768	1.00 20.10
		ATOM	2448		PHE			11.129	36.214	69.070	1.00 21.80 1.00 22.60
		ATOM	2449		PHE			11.337	36.890	66.400	1.00 24.74
40		ATOM	2450		PHE			11.750	37.416	68.716	1.00 27.24
	50	ATOM	2451	CZ	PHE			11.857	37.756	67.368	1.00 27.24
		ATOM	2452	N	TRP			12.235	31.828	68.861	1.00 24.97
		ATOM	2453	CA	TRP			13.639	31.541	69.068	1.00 17.87
		ATOM	2454	c.	TRP			14.292	30.775	67.953	
		ATOM	2455	ŏ	TRP			15.518	30.769	67.830	1.00 28.55 1.00 29.23
45	55	ATOM	2456	СВ	TRP			13.860			
45	<i>J</i> J	ATOM	2457						30.842	70.362	1.00 16.03
		ATOM	2458	CG	TRP TRP			13.613	29.408	70.161	1.00 19.64
		ATOM	2459					12.428	28.787	70.247	1.00 22.39
					TRP			14.599	28.430	69.876	1.00 21.70
	60	ATOM	2460		TRP			12.597	27.457	70.033	1.00 24.22
	UU	ATOM	2461		TRP			13.934	27.205	69.801	1.00 27.96
50		ATOM	2462		TRP			15.976	28.481	69.681	1.00 22.89
JU		ATOM	2463	C22	TRP	A	315	14.631	26.018	69.547	1.00 27.76
		ATOM	2464		TRP			16.651	27.321	69.421	1.00 23.16
		ATOM	2465	CH2	TRP	А	315	15.991	26.108	69.341	1.00 23.94

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5		ATOM	2466	N		A 316		13.488	30.114	67.144	1.00 26.33
		MOTA	2467	CA		A 316		14.092	29.400	66.067	1.00 25.44
		MOTA	2468	С		A 316		14.666	30.443	65.129	1.00 33.21
	_	MOTA	2469	0		A 316		15.737	30.252	64.530	1.00 37.80
	5	MOTA	2470	CB		A 316		13.050	28.567	65.311	1.00 24.82
		ATOM	2471	CG		A 316		12.663	27.242	65.956	1.00 27.62
10		MOTA	2472		LEU I			11.574	26.552	65.106	1.00 22.30
10		ATOM	2473		LEU A			13.897	26.344	66.097	1.00 27.03
	10	MOTA	2474	N		A 317		13.931	31.555	64.997	1.00 20.55
	10	MOTA	2475	CA	ASN A			14.354	32.624	64.115	1.00 19.34
		ATOM	2476	C		A 317		15.603	33.333	64.531	1.00 30.38
		ATOM	2477	0		A 317		16.553	33.425	63.766	1.00 32.04
		ATOM	2478 2479	CB	ASN A			13.273	33.682	63.838	1.00 14.82
15	15	ATOM ATOM	2479	CG OD1		A 317		12.330	33.177	62.793	1.00 31.14
	10	ATOM	2481		ASN A			12.151	31.966	62.657	1.00 38.42
		ATOM	2482	N N				11.724	34.074	62.049	1.00 17.34
		MOTA	2483	CA		A 318 A 318		15.562	33.870	65.750	1.00 26.15
		ATOM	2484	C		A 318		16.624 17.860	34.648	66.358	1.00 20.23
	20	ATOM	2485	ŏ		A 318		19.006	33.884	66.816	1.00 23.53
	20	ATOM	2486	СВ	GLU A			15.998	34.273	66.554	1.00 26.34
20		ATOM	2487	CG		A 318		14.999	35.484	67.456	1.00 19.11
		ATOM	2488	CD		A 318		15.615	36.480 37.391	66.800	1.00 24.06
		ATOM	2489		GLU A					65.758	1.00 40.32
	25	ATOM	2490		GLU A			16.833 14.703	37.559	65.612	1.00 21.24
	20	ATOM	2491	N	GLY A			17.621	38.025 32.782	65.062	1.00 24.23
		ATOM	2492	CA	GLY A			18.681	31.955	67.494	1.00 17.17
25		ATOM	2493	c		A 319		19.673	31.601	68.016 66.953	1.00 15.31
25		MOTA	2494	ŏ		A 319		20.860	31.897	67.080	1.00 24.07
	30	MOTA	2495	N		A 320		19.165	30.956	65.907	1.00 28.47
	-	ATOM	2496	CA	HIS A			19.977	30.556	64.790	1.00 20.24 1.00 20.13
		ATOM	2497	c		A 320		20.678	31.759	64.142	1.00 24.97
		MOTA	2498	ō		A 320		21.855	31.700	63.739	1.00 24.97
		ATOM	2499	СВ	HIS A			19.143	29.737	63.791	1.00 23.54
30	35	ATOM	2500	CG	HIS A			18.662	28.426	64.349	1.00 20.57
•		ATOM	2501		HIS A			17.471	28.332	65.058	1.00 22.37
		ATOM	2502		HIS A			19.217	27.176	64.286	1.00 19.52
		ATOM	2503		HIS A			17.336	27.046	65.385	1.00 19.18
		MOTA	2504		HIS A			18.368	26.329	64.952	1.00 18.12
	40	ATOM	2505	N	THR A			19.958	32.875	64.053	1.00 21.61
		ATOM	2506	CA	THR A			20.543	34.056	63.478	1.00 22.16
35		ATOM	2507	С	THR A			21.697	34.552	64.342	1.00 27.47
		ATOM	2508	0		321		22.789	34.825	63.836	1.00 26.64
		ATOM	2509	CB	THR A			19.470	35.097	63.113	1.00 27.88
	45	MOTA	2510	OG1				18.403	34.392	62.523	1.00 27.92
		MOTA	2511	CG2	THR A	321		19.999	36.088	62.087	1.00 18.05
		ATOM	2512	N	VAL A	322	2	21.496	34.634	65.659	1.00 21.90
40		MOTA	2513	CA	VAL A	322	2	22.610	35.054	66.470	1.00 19.44
40		MOTA	2514	C	VAL A	A 322	2	23.762	34.071	66.285	1.00 24.43
	50	ATOM	2515	0	VAL A	A 322	2	24.926	34.414	66.188	1.00 21.48
		ATOM	2516	CB	VAL A	A 322	2	22.218	35.185	67.928	1.00 20.92
		ATOM	2517	CG1	VAL A	A 322	2	23.406	35.644	68.772	1.00 18.37
		MOTA	2518	CG2	VAL A	A 322	2	21.093	36.200	68.048	1.00 20.01
		ATOM	2519	N	TYR A		2	23.427	32.811	66.197	1.00 27.08
45	55	ATOM	2520	CA.	TYR A	A 323	2	24.446	31.803	66.013	1.00 26.26
		MOTA	2521	С	TYR A		2	25.222	32.036	64.728	1.00 28.26
		MOTA	2522	0	TYR A	A 323	2	26.431	31.894	64.643	1.00 27.51
		MOTA	2523	CB	TYR A			23.804	30.407	66.020	1.00 25.74
		MOTA	2524	CG	TYR A	A 323	2	24.867	29.341	65.987	1.00 26.66
	60	ATOM	2525		TYR A			25.539	28.957	67.150	1.00 29.09
		MOTA	2526		TYR A		2	25.199	28.713	64.789	1.00 24.52
50		MOTA	2527		TYR A			26.530	27.974	67.157	1.00 22.56
		MOTA	2528		TYR A			26.178	27.722	64.770	1.00 25.31
		MOTA	2529	CZ	TYR A	A 323	2	26.846	27.370	65.944	1.00 29.19

5		ATOM	2530	OH	TYR	Α	323	27.823	26.434	65.895	1.00 27.51
		ATOM	2531	N	LEU	Α	324	24.497	32.408	63.702	1.00 24.82
		ATOM	2532	CA	LEU	Α	324	25.135	32.638	62.439	1.00 26.04
	_	ATOM	2533	С	LEU	Α	324	25.832	33.952	62.417	1.00 30.92
	5	ATOM	2534	0	LEU	Α	324	26.903	34.045	61.851	1.00 33.76
		MOTA	2535	СВ	LEU	Α	324	24.176	32.537	61.235	1.00 26.21
		ATOM	2536	CG	LEU	Α	324	23.916	31.112	60.778	1.00 28.46
10		ATOM	2537	CD1	LEU			22.752	31.109	59.791	1.00 28.95
		ATOM	2538		LEU			25.169	30.508	60.151	1.00 26.54
	10	ATOM	2539	N	GLU			25.234	34.976	63.033	1.00 27.04
		ATOM	2540	CA	GLU			25.870	36.303	63.064	1.00 22.88
		ATOM	2541	C	GLU			27.282	36.210	63.624	1.00 28.76
		ATOM	2542	ō	GLU			28.250	36.722	63.026	1.00 26.24
		ATOM	2543	СВ	GLU			25.016	37.365	63.759	1.00 22.01
15	15	ATOM	2544	CG	GLU			25.827	38.411	64.524	1.00 22.01
	10	ATOM	2545	CD	GLU			25.027	39.040		
		ATOM	2546		GLU					65.646	1.00 72.11
								23.866	38.764	65.862	1.00 41.88
		ATOM	2547		GLU			25.719	39.922	66.350	1.00 67.15
	20	ATOM	2548	N	ARG			27.349	35.479	64.755	1.00 27.84
	20	ATOM	2549	CA	ARG			28.551	35.213	65.511	1.00 28.10
20		ATOM	2550	C	ARG			29.604	34.457	64.771	1.00 30.90
		MOTA	2551	0	ARG			30.763	34.747	64.976	1.00 33.93
		MOTA	2552	СВ	ARG			28.334	34.761	66.947	1.00 31.52
	0.5	MOTA	2553	CG	ARG			27.645	35.864	67.726	1.00 22.20
	25	MOTA	2554	CD	ARG	Α	326	27.462	35.572	69.203	1.00 28.71
		ATOM	2555	NE	ARG	Α	326	26.727	36.673	69.830	1.00 23.82
		ATOM	2556	CZ	ARG	Α	326	25.805	36.556	70.780	1.00 26.09
25		ATOM	2557	NH1	ARG	Α	326	25.443	35.388	71.305	1.00 23.16
20		ATOM	2558	NH2	ARG	Α	326	25.220	37.655	71.222	1.00 24.77
	30	ATOM	2559	N	HIS			29.221	33.511	63.918	1.00 29.85
		MOTA	2560	CA	HIS			30.207	32.777	63.120	1.00 30.52
		ATOM	2561	C	HIS			30.778	33.738	62.085	1.00 35.50
		ATOM	2562	ō	HIS			31.966	33.777	61.822	1.00 36.74
		ATOM	2563	СВ	HIS			29.591	31.555	62.407	1.00 30.74
30	35	ATOM	2564	CG	HIS			29.764	30.259	63.176	
50		ATOM	2565		HIS			30.963	29.913		1.00 34.51
		ATOM	2566		HIS			28.875		63.788	1.00 36.17
		ATOM	2567		HIS				29.263	63.432	1.00 35.58
		ATOM	2568		HIS			30.778	28.740	64.384	1.00 35.27
	40	ATOM						29.532	28.322	64.191	1.00 35.56
	טד		2569	N	ILE			29.902	34.549	61.511	1.00 31.10
35		ATOM	2570	CA	ILE			30.328	35.517	60.528	1.00 31.66
33		ATOM	2571	C	ILE			31.416	36.407	61.086	1.00 40.12
		ATOM	2572	0	ILE			32.451	36.615	60.465	1.00 40.81
	46	ATOM	2573	СВ	ILE			29.175	36.379	59.998	1.00 32.94
	45	ATOM	2574		ILE			28.220	35.570	59.114	1.00 29.53
		ATOM	2575		ILE			29.694	37.591	59.201	1.00 30.91
		MOTA	2576		ILE			27.119	36.463	58.535	1.00 32.98
40		ATOM	2577	N	CYS			31.179	36.948	62.266	1.00 37.88
40		ATOM	2578	CA	CYS	Α	329	32.170	37.810	62.851	1.00 39.54
	50	ATOM	2579	С	CYS	Α	329	33.475	37.092	63.157	1.00 40.19
		ATOM	2580	0	CYS	Α	329	34.567	37.642	62.971	1.00 38.44
		ATOM	2581	CB	CYS	A	329	31.607	38.509	64.083	1.00 42.61
		ATOM	2582	SG	CYS			30.241	39.595	63.619	1.00 48.14
		ATOM	2583	N	GLY			33.332	35.852	63.632	1.00 34.74
45	55	ATOM	2584	CA	GLY			34.471	35.030	63.980	1.00 35.20
45		ATOM	2585	С	GLY			35.359	34.854	62.778	1.00 43.66
		ATOM	2586	ŏ	GLY			36.581	34.857	62.891	
		ATOM	2587	N	ARG			34.709	34.725		1.00 46.79
		ATOM	2588	CA	ARG					61.622	1.00 34.99
	60	ATOM	2589					35.416	34.562	60.392	1.00 33.19
	50			C	ARG			36.086	35.863	60.017	1.00 40.63
50		ATOM	2590	O	ARG			37.238	35.914	59.586	1.00 44.40
50		ATOM	2591	CB	ARG			34.494	34.101	59.269	1.00 31.29
		ATOM	2592	CG	ARG			33.987	32.685	59.450	1.00 47.66
		MOTA	2593	CD	ARG	A	331	34.812	31.722	58.622	1.00 70.36

5		MOTA	2594	NE	ARG A 331	34.461	31.851	57.221	1.00 80.25
		ATOM	2595	CZ	ARG A 331	33.615	31.023	56.628	1.00100.00
		MOTA	2596		ARG A 331	33.055	29.999	57.279	1.00 79.12
	_	MOTA	2597	NH2	ARG A 331	33.334	31.216	55.341	1.00 89.33
	5	MOTA	2598	N	LEU A 332	35.342	36.926	60.172	1.00 32.14
		ATOM	2599	CA	LEU A 332	35.885	38.198	59.820	1.00 30.02
		ATOM	2600	С	LEU A 332	37.013	38.612	60.761	1.00 40.33
10		MOTA	2601	0	LEU A 332	38.084	38.972	60.286	1.00 40.10
		MOTA	2602	CB	LEU A 332	34.772	39.262	59.822	1.00 28.20
	10	ATOM	2603	CG	LEU A 332	34.451	39.896	58.469	1.00 28.82
		MOTA	2604	CD1	LEU A 332	35.007	39.063	57.341	1.00 23.73
		ATOM	2605	CD2	LEU A 332	32.947	40.114	58.306	1.00 29.76
		ATOM	2606	N	PHE A 333	36.744	38.557	62.091	1.00 37.69
		ATOM	2607	CA	PHE A 333	37.657	38.997	63.143	1.00 34.12
15	15	ATOM	2608	С	PHE A 333	38.251	37.956	64.035	1.00 37.99
		ATOM	2609	0	PHE A 333	39.015	38.293	64.925	1.00 41.67
		ATOM	2610	CB	PHE A 333	36.970	40.058	64.024	1.00 35.62
		ATOM	2611	CG	PHE A 333	36.209	41.003	63.138	1.00 39.09
		MOTA	2612	CD1	PHE A 333	36.887	41.923	62.332	1.00 43.22
	20	ATOM	2613		PHE A 333	34.818	40.941	63.045	1.00 42.78
20		ATOM	2614		PHE A 333	36.205	42.781	61.464	1.00 44.14
20		ATOM	2615		PHE A 333	34.123	41.806	62.194	1.00 46.56
		ATOM	2616	CZ	PHE A 333	34.814	42.716	61.389	1.00 43.20
		ATOM	2617	N	GLY A 334	37.908	36.706	63.865	1.00 34.36
	25	ATOM	2618	CA	GLY A 334	38.507	35.705	64.763	1.00 32.89
		ATOM	2619	С	GLY A 334	37.582	34.985	65.767	1.00 32.67
		ATOM	2620	ō	GLY A 334	36.641	35.540	66.340	1.00 32.07
25		ATOM	2621	N	GLU A 335	37.908	33.726	66.003	1.00 23.52
20		ATOM	2622	CA	GLU A 335	37.196	32.875	66.931	1.00 23.32
	30	ATOM	2623	C	GLU A 335	37.278	33.384	68.346	1.00 29.15
		ATOM	2624	ō	GLU A 335	36.357	33.124	69.112	1.00 29.13
		ATOM	2625	СВ	GLU A 335	37.782	31.488	66.929	1.00 17.35
		MOTA	2626	CG	GLU A 335	37.041	30.591	67.929	1.00 17.33
		ATOM	2627	CD	GLU A 335	35.642	30.305	67.473	1.00 32.37
30	35	ATOM	2628		GLU A 335	35.093	30.944	66.588	1.00 39.31
		ATOM	2629		GLU A 335	35.080	29.317	68.132	1.00 32.80
		ATOM	2630	N	LYS A 336	38.370	34.077	68.706	1.00 24.53
		ATOM	2631	CA	LYS A 336	38.468	34.609	70.061	1.00 25.38
		ATOM	2632	С	LYS A 336	37.445	35.726	70.169	1.00 35.32
	40	ATOM	2633	0	LYS A 336	36.908	36.004	71.233	1.00 38.14
		ATOM	2634	CB	LYS A 336	39.820	35.199	70.421	1.00 25.45
35		ATOM	2635	CG	LYS A 336	40.871	34.188	70.825	1.00 25.43
		ATOM	2636	CD	LYS A 336	42.207	34.846	71.189	1.00 47.10
		ATOM	2637	CE	LYS A 336	43.325	34.600	70.172	1.00 68.74
	45	ATOM	2638	NZ	LYS A 336	44.566	34.072	70.767	1.00 77.62
		ATOM	2639	N	PHE A 337	37.174	36.364	69.029	1.00 31.52
		ATOM	2640	CA	PHE A 337	36.186	37.442	68.967	1.00 31.32
40		ATOM	2641	С	PHE A 337	34.783	36.869	69.083	1.00 31.73
40		ATOM	2642	0	PHE A 337	33.908	37.424	69.742	1.00 35.53
	50	ATOM	2643	СВ	PHE A 337	36.304	38.336	67.709	1.00 30.04
		ATOM	2644	CG	PHE A 337	35.435	39.589	67.747	1.00 35.16
		ATOM	2645		PHE A 337	35.468	40.459	68.843	1.00 43.88
		ATOM	2646		PHE A 337	34.550	39.893	66.709	1.00 40.16
		ATOM	2647		PHE A 337	34.688	41.617	68.913	1.00 46.18
15	55	ATOM	2648		PHE A 337	33.753	41.040	66.760	
45		ATOM	2649	CZ	PHE A 337	33.830	41.908	67.852	1.00 45.62 1.00 45.57
		ATOM	2650	N	ARG A 338	34.566	35.733	68.452	1.00 45.57
		ATOM	2651	CA	ARG A 338	33.266	35.733		
		ATOM	2652	c	ARG A 338	32.944	34.759	68.508	1.00 25.23
	60	ATOM	2653	ò	ARG A 338	31.854		69.922	1.00 29.77
		ATOM	2654	СВ	ARG A 338	33.186	35.025	70.415	1.00 31.81
50		ATOM	2655	CG	ARG A 338	31.839	33.920	67.606	1.00 24.04
50		ATOM	2656	CD	ARG A 338	31.839	33.228	67.623	1.00 21.31
		ATOM	2657	NE	ARG A 338		32.086	66.599	1.00 30.62
		TON	2007	115	WG V 220	32.518	30.892	67.040	1.00 29.87

5		ATOM	2658	CZ	ARG	А	338	31.919	29.781	67.466	1.00 26.37
		ATOM	2659		ARG			30.616	29.687	67.518	1.00 20.26
		ATOM	2660		ARG			32.632	28.737	67.864	1.00 18.57
		ATOM	2661	N	HIS			33.934	34.190	70.577	1.00 25.88
	5	ATOM	2662	CA.	HIS			33.813	33.797	71.982	1.00 25.59
		ATOM	2663	С	HIS			33.455	34.972	72.892	1.00 27.61
		ATOM	2664	0	HIS			32.615	34.912	73.793	1.00 25.27
10		ATOM	2665	CB	HIS			35.065	33.045	72.462	1.00 25.06
		ATOM	2666	CG	HIS			34.923	31.587	72.155	1.00 28.13
	10	ATOM	2667		HIS			35.049	30.612	73.127	1.00 30.52
		ATOM	2668		HIS			34.586	30.970	70.981	1.00 30.89
		ATOM	2669		HIS			34.843	29.442	72.535	1.00 30.89
		ATOM	2670		HIS			34.546	29.616	71.245	1.00 31.36
		ATOM	2671	N	PHE			34.103	36.065	72.608	1.00 24.54
15	15	ATOM	2672	CA	PHE			33.892	37.278	73.334	1.00 25.36
		ATOM	2673	C	PHE			32.452	37.762	73.216	1.00 32.47
		ATOM	2674	ō	PHE			31.822	38.222	74.190	1.00 32.78
		ATOM	2675	СВ	PHE			34.876	38.309	72.801	1.00 26.03
		ATOM	2676	CG	PHE			34.654	39.671	73.346	1.00 26.47
	20	ATOM	2677		PHE			35.238	40.047	74.559	1.00 24.59
		ATOM	2678		PHE			33.902	40.592	72.616	1.00 28.22
20		ATOM	2679		PHE			35.063	41.330	75.072	1.00 21.58
		ATOM	2680		PHE			33.715	41.879	73.115	1.00 29.13
		ATOM	2681	CZ	PHE			34.280	42.225	74.345	1.00 25.28
	25	ATOM	2682	N	ASN			31.944	37.663	72.004	1.00 28.41
		ATOM	2683	CA	ASN			30.600	38.084	71.728	1.00 29.60
		ATOM	2684	c	ASN			29.665	37.110	72.379	1.00 29.00
25		ATOM	2685	ŏ	ASN			28.699	37.511	73.029	1.00 38.32
25		ATOM	2686	CB	ASN			30.322	38.274	70.224	1.00 30.01
	30	ATOM	2687	CG	ASN			31.159	39.374	69.587	1.00 52.80
	••	ATOM	2688		ASN			31.528	39.284	68.404	1.00 52.80
		ATOM	2689		ASN			31.442	40.427	70.359	1.00 41.02
		ATOM	2690	N	ALA			29.994	35.826	72.239	1.00 28.24
		ATOM	2691	CA	ALA			29.195	34.800	72.877	1.00 26.95
30	35	ATOM	2692	c	ALA			29.013	35.134	74.393	1.00 20.93
	••	ATOM	2693	ŏ	ALA			27.877	35.261	74.897	1.00 35.98
		ATOM	2694	СВ	ALA			29.837	33.422	72.671	1.00 35.09
		ATOM	2695	N	LEU			30.153	35.304	75.122	1.00 29.16
		ATOM	2696	CA	LEU			30.162	35.633	76.560	1.00 22.58
	40	ATOM	2697	C	LEU			29.310	36.854	76.831	1.00 27.48
		ATOM	2698	ŏ	LEU			28.452	36.821	77.696	1.00 27.48
35		ATOM	2699	СВ	LEU			31.583	35.786	77.147	1.00 32.73
		ATOM	2700	CG	LEU			31.647	35.693	78.671	1.00 20.08
		ATOM	2701		LEU			30.842	34.510	79.204	1.00 20.08
	45	ATOM	2702		LEU			33.091	35.522	79.111	1.00 17.76
	,,,	MOTA	2703	N	GLY			29.512	37.936	76.080	1.00 22.60
		ATOM	2704	CA	GLY			28.670	39.146	76.278	1.00 24.15
		ATOM	2705	c .	GLY			27.157	38.824	76.136	1.00 31.38
40		ATOM	2706	ŏ	GLY			26.339	39.260	76.943	
	50	ATOM	2707	N	GLY			26.806	38.017	75.094	1.00 32.44
	••	ATOM	2708	CA	GLY			25.451	37.587	74.801	1.00 22.79
		ATOM	2709	c	GLY			24.787	36.994	76.034	1.00 19.88
		ATOM	2710	ō	GLY			23.632	37.294		
		ATOM	2711	N	TRP			25.547	36.153	76.325	1.00 27.56
45	55	ATOM	2712	CA	TRP			25.082	35.520	76.765	1.00 25.41
45	-	ATOM	2713	Ç	TRP			24.825		77.994	1.00 23.90
		ATOM	2714	Ö	TRP				36.541	79.071	1.00 31.54
		ATOM	2715	СВ	TRP			23.957 26.122	36.379	79.924	1.00 29.57
		ATOM	2716	CG	TRP				34.556	78.562	1.00 21.53
	60	ATOM	2717		TRP			25,680	33.880	79.837	1.00 21.92
	50	ATOM	2718		TRP			25.933	34.335	81.079	1.00 24.36
50		ATOM	2719		TRP			25.004	32.597	80.010	1.00 20.97
50		ATOM	2720					25.450	33.453	82.008	1.00 23.95
		ATOM	2721		TRP			24.859	32.388	81.391	1.00 24.13
		VION	2121	CES	TRP	А	340	24.488	31.611	79.144	1.00 21.46

5		MOTA	2722	CZ2	TRP P	346	24.225	31.244	81.921	1.00 22.89
		MOTA	2723	CZ3	TRP A	346	23.872	30.477	79.662	1.00 22.03
		ATOM	2724	CH2	TRP A	346	23.747	30.286	81.046	1.00 21.87
		ATOM	2725	N	GLY A	347	25.627	37.593	79.039	1.00 29.66
	5	ATOM	2726	CA	GLY A	347	25.465	38.625	80.042	1.00 29.03
		ATOM	2727	С	GLY A	347	24.156	39.333	79.844	1.00 33.01
		MOTA	2728	0	GLY A		23.491	39.647	80.799	1.00 34.17
10		ATOM	2729	N	GLU A		23.797	39.574	78.581	1.00 30.57
		MOTA	2730	CA	GLU A		22.535	40.220	78.250	1.00 29.17
	10	ATOM	2731	С	GLU A		21.423	39.282	78.664	1.00 31.25
		ATOM	2732	0	GLU A		20.373	39.663	79.142	1.00 33.71
		ATOM	2733	CB	GLU A		22.432	40.606	76.757	1.00 30.33
		MOTA	2734	CG	GLU A		23.432	41.715	76.336	1.00 49.41
		ATOM	2735	CD	GLU A		23.209	43.088	76.964	1.00 73.39
15	15	ATOM	2736		GLU A		22.295	43.846	76.656	1.00 71.22
		ATOM	2737		GLU A		24.119	43.395	77.857	1.00 44.23
		ATOM	2738	N	LEU A		21.682	38.011	78.541	1.00 27.36
		ATOM	2739	CA	LEU A		20.677	37.081	78.976	1.00 26.89
		ATOM	2740	C	LEU A		20.429	37.250	80.485	1.00 24.87
	20	ATOM	2741	0	LEU A		19.299	37.403	80.914	1.00 28.31
20		ATOM	2742	СВ	LEU A		20.984	35.630	78.529	1.00 27.18
20		ATOM	2743	CG	LEU A		19.943	34.565	78.942	1.00 27.10
		MOTA	2744		LEU A		18.611	34.704	78.154	1.00 30.09
		ATOM	2745		LEU A		20.541	33.169	78.749	1.00 27.10
	25	ATOM	2746	N	GLN A		21.460	37.255	81.315	1.00 27.10
		ATOM	2747	CA	GLN A		21.188	37.428	82.727	1.00 14.70
		ATOM	2748	С	GLN A		20.442	38.722	82.953	1.00 25.53
25		ATOM	2749	ō	GLN A		19.495	38.833	83.737	1.00 28.35
20		ATOM	2750	СВ	GLN A		22.469	37.369	83.536	1.00 22.22
	30	ATOM	2751	CG	GLN A		23.512	36.426	82.919	1.00 22.22
		ATOM	2752	CD	GLN A		24.871	36.673	83.547	1.00 34.49
		ATOM	2753		GLN A		25.261	35.932	84.417	1.00 24.01
		ATOM	2754		GLN A		25.588	37.727	83.127	1.00 36.58
		ATOM	2755	N	ASN A		20.838	39.696	82.201	1.00 22.64
30	35	ATOM	2756	CA	ASN A		20.163	40.960	82.273	1.00 26.10
		ATOM	2757	c	ASN A		18.661	40.780	82.083	1.00 20.10
		ATOM	2758	ŏ	ASN A		17.890	41.098	82.977	1.00 37.43
		ATOM	2759	CB	ASN A		20.769	42.021	81.341	1.00 20.74
		ATOM	2760	CG	ASN A		22.118	42.477	81.847	1.00 23.25
	40	ATOM	2761		ASN A		22.692	41.875	82.771	1.00 26.88
	• • •	ATOM	2762		ASN A		22.644	43.530	81.247	1.00 20.00
35		ATOM	2763	N	SER A		18.228	40.252	80.938	1.00 32.84
		ATOM	2764	CA	SER A		16.784	40.041	80.715	1.00 32.04
		ATOM	2765	ç	SER A		16.107	39.135	81.784	1.00 31.72
	45	ATOM	2766	ŏ	SER A		14.927	39.266	82.189	1.00 28.64
		ATOM	2767	СВ	SER A		16.503	39.531	79.301	1.00 42.57
		ATOM	2768	OG	SER A		17.506	39.979	78.407	1.00 49.17
40		ATOM	2769	N	VAL A		16.874	38.188	82.247	1.00 49.17
40		ATOM	2770	CA	VAL A		16.322	37.351	83.234	1.00 22.13
	50	ATOM	2771	С	VAL A		16.068	38.122	84.516	1.00 36.22
		ATOM	2772	ō	VAL A		14.958	38.076	85.052	1.00 30.22
		ATOM	2773	ÇВ	VAL A		17.137	36.070	83.419	1.00 20.84
		ATOM	2774		VAL A		16.632	35.256	84.634	1.00 15.06
		MOTA	2775		VAL A		16.968	35.284	82.105	
45	55	ATOM	2776	N	LYS A		17.086	38.847	85.002	1.00 20.93 1.00 30.67
40		ATOM	2777	CA	LYS A		16.880	39.587		
		ATOM	2778	C	LYS A		15.660		86.221 86.098	1.00 31.71
		ATOM	2779	õ	LYS A		14.808	40.474		1.00 36.17
		ATOM	2780	СВ	LYS A			40.582	86.980	1.00 35.80
	60	ATOM	2781	CG	LYS A		18.099	40.396	86.624	1.00 35.28
	00	ATOM	2782	CD	LYS A		17.841	41.303	87.818	1.00 51.51
50		ATOM	2783	CE			19.038	41.405	88.749	1.00 60.46
50		ATOM	2783		LYS A		19.198	42.780	89.383	1.00 50.09
		ATOM	2785	NZ N	LYS A		20.596	43.133	89.657	1.00 63.77
		ATOM	2/03	14	THR A	, 333	15.608	41.108	84.962	1.00 32.63

5		ATOM	2786	CA	THR A	355	14.562	42.025	84.610	1.00 34.03
		MOTA	2787	c ·	THR A		13.129	41.422	84.578	1.00 42.11
		ATOM	2788	0	THR A		12.216	42.006	85.154	1.00 40.96
	_	ATOM	2789	CB	THR A	355	14.974	42.736	83.308	1.00 41.11
	5	ATOM	2790	OG1	THR A	355	16.071	43.615	83.542	1.00 29.85
		ATOM	2791	CG2	THR A	355	13.798	43.438	82.656	1.00 45.50
		ATOM	2792	N	PHE A	356	12.895	40.273	83.908	1.00 33.89
10		ATOM	2793	CA	PHE A	356	11.556	39.729	83.860	1.00 29.29
		ATOM	2794	С	PHE A	356	11.209	39.070	85.147	1.00 31.93
	10	MOTA	2795	0	PHE A	356	10.089	39.152	85.642	1.00 33.85
		MOTA	2796	CB	PHE A	356	11.460	38.645	82.785	1.00 33.30
		ATOM.	2797	CG	PHE A	356	11.187	39.196	81.416	1.00 36.54
		ATOM	2798	CD1	PHE A	356	10.106	40.054	81.224	1.00 42.38
15		MOTA	2799	CD2	PHE A	356	11.985	30.858	80.320	1.00 38.62
15	15	ATOM	2800		PHE A		9.831	40.596	79.968	1.00 44.75
		ATOM	2801	CE2	PHE A	356	11.723	39.384	79.055	1.00 43.46
		ATOM	2802	CZ	PHE A	356	10.649	40.261	78.890	1.00 43.86
		ATOM	2803	N	GLY A	357	12.212	38.386	85.661	1.00 30.41
		ATOM	2804	CA	GLY A	357	12.152	37.564	86.864	1.00 29.17
	20	ATOM	2805	С	GLY A	357	12.446	36.100	86.438	1.00 28.92
20		ATOM	2806	0	GLY A	357	12.008	35.642	85.372	1.00 27.33
20		ATOM	2807	N	GLU A	358	13.211	35.382	87.243	1.00 21.27
		ATOM	2808	CA	GLU A	358	13.590	34.040	86.898	1.00 23.10
		MOTA	2809	С	GLU A	358	12.424	33.104	86.747	1.00 31.53
	25	MOTA	2810	0	GLU A	358	12.581	31.972	86.294	1.00 30.92
		ATOM	2811	CB	GLU A	358	14.596	33.473	87.880	1.00 25.36
		ATOM	2812	CG	GLU A	358	14.011	33.436	89.301	1.00 38.73
25		MOTA	2813	CD	GLU A	358	15.011	33.037	90.345	1.00 56.34
		ATOM	2814	OE1	GLU A	358	16.026	32.446	90.071	1.00 50.55
	30	MOTA	2815	OE2	GLU A	358	14.678	33.403	91.564	1.00 75.65
		MOTA	2816	N	THR A	359	11.246	33.542	87.139	1.00 27.87
		MOTA	2817	CA	THR A	359	10.154	32.625	86.970	1.00 25.66
		MOTA	2818	С	THR A	359	9.236	33.152	85.906	1.00 25.96
		ATOM	2819	0	THR A	359	8.247	32.528	85.533	1.00 25.58
30	35	MOTA	2820	CB	THR A	359	9.423	32.341	88.253	1.00 25.00
		MOTA	2821	OG1	THR A	359	8.908	33.565	88.692	1.00 33.10
		ATOM	2822	CG2	THR A	359	10.406	31.785	89.273	1.00 14.43
		ATOM	2823	N	HIS A	360	9.602	34.310	85.407	1.00 20.75
	40	ATOM	2824	CA	HIS A		8.837	34.902	84.363	1.00 22.77
	40	ATOM	2825	С	HIS A	360	8.823	34.034	83.130	1.00 35.30
25		MOTA	2826	0	HIS A		9.858	33.611	82.620	1.00 37.42
35		ATOM	2827	CB	HIS A		9.294	36.291	83.982	1.00 23.18
		ATOM	2828	CG	HIS A		8.207	36.908	83.219	1.00 27.05
	40	ATOM	2829		HIS A		7.532	38.009	83.691	1.00 29.34
	45	MOTA	2830		HIS A		7.651	36.545	82.059	1.00 29.91
		MOTA	2831		HIS A		6.596	38.315	82.806	1.00 27.94
		MOTA	2832		HIS A		6.651	37.440	81.812	1.00 29.60
40		ATOM	2833	N	PRO A		7.606	33.817	82.666	1.00 32.40
	50	ATOM	2834	CA	PRO A		7.301	32.999	81.519	1.00 29.46
	50	ATOM	2835	С	PRO A		7.862	33.478	80.224	1.00 30.59
		ATOM	2836	0	PRO A		7.907	32.737	79.248	1.00 33.00
		MOTA	2837	СВ	PRO A		5.770	32.963	81.478	1.00 30.74
		MOTA	2838	CG	PRO A		5.311	33.172	82.927	1.00 34.96
	E E	MOTA	2839	CD	PRO A		6.463	33.869	83.627	1.00 31.82
45	55	ATOM	2840	N	PHE A		8.289	34.712	80.179	1.00 26.32
		MOTA	2841	CA	PHE A		8.823	35.173	78.933	1.00 25.68
		MOTA	2842	С	PHE A		10.261	34.781	78.829	1.00 29.73
		MOTA	2843	0	PHE A		10.906	35.131	77.870	1.00 32.02
	60	MOTA	2844	CB	PHE A		8.643	36.677	78.723	1.00 28.12
	60	MOTA	2845	CG	PHE A		7.194	37.105	78.629	1.00 30.03
		MOTA	2846		PHE A		6.204	36.276	78.098	1.00 30.92
50		MOTA	2847		PHE A		6.804	38.372	79.051	1.00 32.04
		MOTA	2848		PHE A		4.864	36.655	77.998	1.00 26.59
		MOTA	2849	CE2	PHE A	362	5.470	38.773	78.952	1.00 32.40

5		ATOM	2850	CZ	PHE A	362	4.495	37.920	78.435	1.00 26.37
		MOTA	2851	N .	THR A		10.730	34.049	79.843	
		ATOM	2852	CA	THR A		12,102	33.575		1.00 27.22
		ATOM	2853	c .	THR A		12.251		79.943	1.00 27.52
	5	ATOM	2854	ŏ	THR A		13.331	32.132	79.504	1.00 29.28
	•	ATOM	2855	СВ	THR A			31.560	79.524	1.00 29.42
		ATOM	2856				12.697	33.777	81.360	1.00 31.67
10		ATOM	2857		THR A		12.279	32.745	82.218	1.00 26.17
10					THR A		12.278	35.118	81.930	1.00 31.62
	10	ATOM	2858	N	LYS A		11.148	31.530	79.113	1.00 23.08
	10	ATOM	2859		LYS A		11.174	30.160	78.664	1.00 20.50
		MOTA	2860		LYS A		11.556	30.270	77.217	1.00 28.83
		ATOM	2861	0	LYS A		11.139	31.239	76.570	1.00 29.80
		MOTA	2862	CB	LYS A		9.766	29.584	78.667	1.00 23.55
	1.5	ATOM	2863	CG	LYS A	364	9.252	29.134	80.022	1.00 40.85
15	15	ATOM	2864	CD	LYS A	364	7.761	29.369	80.162	1.00 44.83
		MOTA	2865	CE	LYS A	364	7.131	28.492	81.224	1.00 66.38
		ATOM	2866	NZ	LYS A	364	6.063	27.638	80.691	1.00 91.70
		ATOM	2867	N	LEU A	365	12.332	29.328	76.698	1.00 23.57
		MOTA	2868		LEU A		12.699	29.420	75.312	1.00 23.95
	20	ATOM	2869		LEU A		11.414	29.419	74.445	
		ATOM	2870		LEU A		11.166	30.369		1.00 35.57
20		ATOM	2871		LEU A		13.702		73.708	1.00 34.58
		MOTA	2872		LEU A			28.303	75.021	1.00 25.08
		ATOM	2873		LEU A		14.456	28.372	73.702	1.00 31.15
	25	ATOM	2874				14.987	29.778	73.466	1.00 33.16
	23	ATOM			LEU A		15.609	27.353	73.781	1.00 30.62
			2875		VAL A		10.572	28.360	74.564	1.00 35.62
		ATOM	2876		VAL A		9.294	28.232	73.840	1.00 32.10
25		ATOM	2877		VAL A		8.211	28.911	74.694	1.00 33.14
	20	ATOM	2878		VAL A		7.982	28.470	75.808	1.00 34.20
	30	ATOM	2879		VAL A		8.936	26.739	73.568	1.00 34.73
		ATOM	2880		VAL A		7.558	26.605	72.933	1.00 34.88
		MOTA	2881	CG2	VAL A	366	9.922	26.012	72.649	1.00 32.65
		ATOM	2882	N '	VAL A	367	7.562	29.990	74.211	1.00 28.76
		ATOM	2883	CA '	VAL A	367	6.532	30.700	74.987	1.00 28.27
30	35	MOTA	2884	C '	VAL A	367	5.161	30.613	74.420	1.00 30.62
		ATOM	2885	0 '	VAL A	367	4.994	30.509	73.235	1.00 34.30
		ATOM	2886		VAL A		6.773	32.185	75.061	1.00 33.45
		ATOM	2887		VAL A		8.178	32.478	75.565	1.00 33.43
		ATOM	2888		VAL A		6.498	32.804	73.693	1.00 33.18
	40	ATOM	2889		ASP A		4.168	30.722	75.290	
		ATOM	2890		ASP A		2.764	30.771	74.984	1.00 29.27
35		ATOM	2891		ASP A		2.315			1.00 27.67
		ATOM	2892		ASP A		2.283	32.207	74.862	1.00 26.94
		ATOM	2893		ASP A			32.975	75.830	1.00 23.11
	45	ATOM	2894		ASP A		1.990	30.073	76.100	1.00 26.80
		ATOM	2895		ASP A		0.572	29.781	75.613	1.00 37.90
		ATOM	2896	ODI I	MOP A	300	0.276	30.123	74.481	1.00 38.93
					ASP A		-0.215	29.217	76.380	1.00 38.59
40		ATOM	2897		LEU A		2.027	32.588	73.622	1.00 26.55
••	50	ATOM	2898		LEU A		1.643	33.953	73.373	1.00 27.39
	50	ATOM	2899		LEU A		0.138	34.105	73.301	1.00 30.74
		ATOM	2900		LEU A		~0.372	34.979	72.648	1.00 30.68
		ATOM	2901		LEU A	369	2.281	34.395	72.064	1.00 26.06
		ATOM	2902	CG]	LEU A	369	3.759	34.760	72.229	1.00 26.80
	~ ~	ATOM	2903	CD1 1	LEU A	369	4.343	35.415	70.994	1.00 24.30
45	55	ATOM	2904	CD2 1	LEU A	369	4.014	35.728	73.384	1.00 21.81
40		ATOM	2905		THR A		-0.577	33.154	73.953	1.00 30.26
		ATOM	2906	CA 7	THR A	370	-2.022	33.306	74.093	
		ATOM	2907		THR A		-2.355	34.519	74.941	1.00 31.38
		ATOM	2908		THR A		-1.821	34.714		1.00 38.62
	60	ATOM	2909		THR A		-2.601	32.056	76.027 74.750	1.00 38.84
		ATOM	2910		THR A		-2.472	30.949		1.00 34.04
50		ATOM	2911		THR A		-4.091		73:873	1.00 29.99
50		ATOM	2912		ASP A			32.266	75.052	1.00 26.40
		ATOM	2913				-3.173	35.387	74.363	1.00 37.89
		AI OIT	7313	CA A	ASP A	3/1	-3.641	36.612	75.012	1.00 37.85

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5		MOTA	2914	C,	ASP A		-2.557	37.636	75.255	1.00 40.92
		MOTA	2915	0	ASP A		-2.784	38.625	75.933	1.00 41.63
		MOTA	2916	CB	ASP A	371	-4.519	36.375	76.245	1.00 39.88
	_	MOTA	2917	CG	ASP A	371	-5.805	35.733	75.798	1.00 51.30
	5	MOTA	2918	ODJ	. ASP A	371	-6.373	36.072	74.761	1.00 50.39
		MOTA	2919	OD2	ASP A	371	-6.206	34.754	76.583	1.00 48.61
		ATOM	2920	N	ILE A		-1.387	37.398	74.664	1.00 36.37
10		ATOM	2921	CA	ILE A		-0.259	38.283	74.817	1.00 34.61
		ATOM	2922	С	ILE A		0.203	39.018	73.555	1.00 35.46
	10	ATOM	2923	ō	ILE A		0.545	38.400	72.548	
		ATOM	2924	СB	ILE A		0.920	37.511	75.381	1.00 36.69
		ATOM	2925		ILE A		0.658	37.195		1.00 36.51
		ATOM	2926		ILE A		2.121		76.842	1.00 37.01
		ATOM	2927		ILE A			39.441	75.281	1.00 35.52
15	15	ATOM	2928	N	ASP A		1.268	38.261	77.747	1.00 54.33
	10	ATOM	2929	CA			0.254	40.345	73.601	1.00 25.92
		ATOM	2930	C	ASP A		0.747	41.053	72.450	1.00 23.77
					ASP A		2.263	40.781	72.360	1.00 31.40
		ATOM	2931	0	ASP A		3.040	41.002	73.305	1.00 32.80
	20	ATOM	2932	CB	ASP A		0.408	42.543	72.519	1.00 25.08
	20	ATOM	2933	CG	ASP A		1.064	43.356	71.418	1.00 43.24
20		ATOM	2934		ASP A		1.861	42.894	70.616	1.00 45.30
		MOTA	2935	OD2	ASP A		0.668	44.610	71.395	1.00 38.59
		MOTA	2936	N	PRO A	374	2.709	40.267	71.225	1.00 29.51
	0.5	MOTA	2937	CA	PRO A	374	4.123	39.943	71.132	1.00 28.52
	25	ATOM	2938	C	PRO A	374	5.029	41.090	71.506	1.00 32.54
		ATOM	2939	0	PRO A	374	6.019	40.905	72.217	1.00 29.62
		ATOM	2940	CB	PRO A	374	4.390	39.421	69.714	1.00 28.88
25		ATOM	2941	CG	PRO A	374	3.028	39.278	69.032	1.00 32.27
		ATOM	2942	CD	PRO A	374	1.966	39.786	70.008	1.00 28.84
	30	ATOM	2943	N	ASP A	375	4.660	42.257	70.981	1.00 26.85
		ATOM	2944	CA	ASP A		5.357	43.511	71.154	1.00 24.25
		ATOM	2945	С	ASP A		5.695	43.783	72.628	1.00 33.10
		ATOM	2946	0	ASP A		6.648	44.494	72.988	1.00 30.67
		ATOM	2947	СВ	ASP A		4.507	44.617	70.509	1.00 24.46
30	35	ATOM	2948	CG	ASP A		4.753	44.836	69.033	1.00 24.46
		ATOM	2949		ASP A		5.703	44.393	68.411	
		ATOM	2950		ASP A		3.852	45.609	68.491	1.00 33.47
		ATOM	2951	N	VAL A		4.885	43.161		1.00 38.41
		ATOM	2952	CA	VAL A		5.001		73.477	1.00 30.21
	40	ATOM	2953	C.	VAL A			43.232	74.904	1.00 25.40
		ATOM	2954	ō	VAL A		5.879	42.106	75.431	1.00 37.27
35		ATOM	2955	СВ			6.599	42.299	76.394	1.00 42.46
		ATOM	2956		VAL A		3.638	43.099	75.550	1.00 22.48
		ATOM			VAL A		3.799	42.533	76.975	1.00 21.25
	45		2957		VAL A		2.926	44.440	75.547	1.00 18.29
	72	ATOM	2958	N	ALA A		5.811	40.905	74.831	1.00 30.48
		ATOM	2959	CA	ALA A		6.671	39.79 3	75.288	1.00 27.04
		ATOM	2960	C	ALA A		8.149	39.911	74.797	1.00 28.15
40		ATOM	2961	0	ALA A		9.077	39.325	75.312	1.00 27.36
,,,	50	ATOM	2962	CB	ALA A		6.091	38.433	74.891	1.00 26.74
	50	ATOM	2963	N	TYR A	378	8.376	40.692	73.768	1.00 25.81
		ATOM	2964	CA	TYR A	378	9.683	40.876	73.161	1.00 25.43
		ATOM	2965	С	TYR A	378	10.862	41.194	74.057	1.00 30.49
		ATOM	2966	0	TYR A	378	10.873	42.204	74.747	1.00 32.35
		ATOM	2967	CB	TYR A	378	9.549	41.924	72.068	1.00 26.20
45	55	ATOM	2968	CG	TYR A	378	10.804	42.168	71.327	1.00 19.90
40		ATOM	2969	CD1	TYR A	378	11.256	41.231	70.406	1.00 18.53
		ATOM	2970		TYR A		11.536	43.331	71.543	1.00 18.47
		ATOM	2971		TYR A		12.444	41.436	69.716	
		ATOM	2972		TYR A		12.719	43.555	70.840	1.00 15.98
	60	ATOM	2973	CZ	TYR A		13.161	42.609		1.00 18.77
		ATOM	2974	ОН	TYR A		14.309		69.920	1.00 16.37
50		ATOM	2975	N	SER A		11.879	42.811	69.212	1.00 32.30
50		ATOM	2976	CA	SER A		13.115	40.317	73.977	1.00 23.03
		ATOM	2977	C	SER A		14.267	40.430	74.725	1.00 18.13
				-	JUN A	213	14.20/	39.777	73.970	1.00 20.60

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5		ATOM	2978	Ο,	SER A	379	14.100	39.334	72.843	1.00 18.46
		ATOM	2979	CB	SER A		12.976	39.740	76.067	1.00 23.56
		MOTA	2980	OG	SER A		12.805	38.329	75.883	1.00 37.26
	_	MOTA	2981	N	SER A		15.424	39.697	74.651	1.00 23.65
	5	ATOM	2982	CA	SER A		16.701	39.084	74.222	1.00 26.09
		ATOM	2983	C	SER A		16.669	37.571	74.457	1.00 28.37
10		ATOM	2984	0	SER A		17.480	36.785	73.975	1.00 30.81
70		MOTA	2985	CB	SER A		17.889	39.588	75.062	1.00 31.60
	10	ATOM	2986	OG	SER A		18.036	41.000	75.033	1.00 42.48
	10	ATOM	2987	N	VAL A		15.718	37.188	75.260	1.00 18.04
		ATOM	2988 2989	CA	VAL A		15.595	35.812	75.598	1.00 14.91
		ATOM ATOM	2990	C O	VAL A		15.708	34.897	74.419	1.00 20.31
		ATOM	2991	CB	VAL A		16.620	34.091	74.330	1.00 27.64
15	15	ATOM	2992		VAL A		14.408	35.546	76.501	1.00 16.34
	10	ATOM	2993		VAL A		14.284	34.062	76.734	1.00 17.26
		ATOM	2994	N	PRO A		14.687 14.797	36.204	77.829	1.00 13.94
		ATOM	2995	CA	PRO A		14.886	35.005 34.139	73.489	1.00 16.53
		ATOM	2996	c	PRO A		16.222		72.324	1.00 17.21
	20	ATOM	2997	ō	PRO A		16.709	34.230 33.192	71.634	1.00 24.01
		ATOM	2998	СВ	PRO A		13.777	34.514	71.207 71.351	1.00 27.79
20		ATOM	2999	CG	PRO A		13.003	35.618	72.033	1.00 17.20
		MOTA	3000	CD	PRO A		13.627	35.873	73.399	1.00 18.32 1.00 12.12
		ATOM	3001	N	TYR A		16.809	35.447	71.542	1.00 12.12
	25	ATOM	3002	CA	TYR A		18.112	35.648	70.902	1.00 19.33
		ATOM	3003	С	TYR A		19.246	34.953	71.651	1.00 28.79
		ATOM	3004	0	TYR A		19.980	34.117	71.104	1.00 31.38
25		ATOM	3005	CB	TYR A	383	18.468	37.135	70.894	1.00 21.02
		ATOM	3006	CG	TYR A	383	17.593	37.968	70.011	1.00 23.86
	30	ATOM	3007	CD1	TYR A	383	16.290	38.277	70.404	1.00 28.36
		ATOM	3008		TYR A		18.067	38.450	68.784	1.00 20.93
		ATOM	3009		TYR A		15.473	39.054	69.576	1.00 30.88
		ATOM	3010	CE2	TYR A	383	17.272	39.244	67.957	1.00 18.71
202	25	ATOM	3011	CZ	TYR A		15.967	39.533	68.358	1.00 25.95
30	35	ATOM	3012	ОН	TYR A		15.171	40.294	67.556	1.00 30.84
		ATOM	3013	N	GLU A		19.389	35.333	72.921	1.00 20.17
		ATOM	3014	CA	GLU A		20.419	34.857	73.803	1.00 17.57
		ATOM	3015	С	GLU A		20.188	33.506	74.405	1.00 22.88
	40	ATOM	3016	0	GLU A		21.151	32.775	74.669	1.00 25.65
	40	ATOM	3017	CB	GLU A		20.833	35.973	74.773	1.00 20.44
35		ATOM ATOM	3018 3019	CG	GLU A		21.263	37.202	73.944	1.00 15.21
		ATOM	3020	CD	GLU A		22.539	36.937	73.184	1.00 26.58
		ATOM	3021		GLU A		23.185	35.915	73.293	1.00 17.84
	45	ATOM	3022	N	LYS A		22.887	37.915	72.400	1.00 21.88
		ATOM	3023	CA	LYS A		18.935 18.736	33.116 31.767	74.610	1.00 20.33
		ATOM	3024	c c	LYS A		18.865	30.716	75.146	1.00 20.05
		ATOM	3025	ŏ	LYS A		19.420	29.621	74.028 74.219	1.00 27.19
40		ATOM	3026	CB	LYS A		17.507	31.577	76.014	1.00 31.66
	50	ATOM	3027	CG	LYS A		17.676	30.384	76.953	1.00 21.51 1.00 22.29
		ATOM	3028	CD	LYS A		16.386	29.820	77.518	1.00 22.29
		ATOM	3029	CE	LYS A		16.049	30.277	78.937	1.00 31.60
		ATOM	3030	NZ	LYS A		14.783	29.694	79.441	1.00 30.38
		ATOM	3031	N	GLY A		18.364	31.084	72.832	1.00 20.72
45	55	ATOM	3032	CA	GLY A		18.453	30.248	71.637	1.00 17.41
		ATOM	3033	С	GLY A		19.924	30.106	71.298	1.00 20.81
		ATOM	3034	0	GLY A		20.396	29.001	71.225	1.00 22.50
		ATOM	3035	N	PHE A		20.683	31.228	71.163	1.00 20.30
	40	ATOM	3036	CA	PHE A		22.137	31.158	70.900	1.00 19.92
	60	ATOM	3037	С	PHE A		22.840	30.263	71.905	1.00 29.09
		ATOM	3038	0	PHE A	387	23.685	29.478	71.530	1.00 32.80
50		ATOM	3039	CB	PHE A		22.852	32.519	70.955	1.00 20.07
		ATOM	3040	CG	PHE A	387	24.344	32.358	70.872	1.00 19.41
		ATOM	3041	CD1	PHE A	387	24.949	32.163	69.631	1.00 19.67

_			2040							
5		ATOM	3042		PHE A		25.157	32.373	72.007	1.00 25.27
		MOTA	3043		PHE A		26.329	31.977	69.525	1.00 20.88
		ATOM	3044		PHE A		26.542	32.202	71.916	1.00 28.83
	5	MOTA	3045	CZ	PHE A		27.131	31.981	70.668	1.00 23.24
	,	MOTA MOTA	3046	N	ALA A		22.495	30.381	73.203	1.00 25.48
			3047	CA	ALA A		23.133	29.556	74.242	1.00 23.14
10		MOTA	3048	C	ALA A		22.872	28.108	74.055	1.00 32.10
.•		MOTA	3049	0	ALA A		23.757	27.282	74.258	1.00 37.82
	10	ATOM	3050	CB	ALA A		22.717	29.932	75.633	1.00 23.02
	IO	MOTA	3051	N.	LEU A		21.636	27.793	73.691	1.00 26.31
		MOTA	3052	CA	LEU A		21.275	26.405	73.460	1.00 21.42
		ATOM ATOM	3053 3054	C	LEU A		22.189	25.906	72.372	1.00 27.91
		ATOM	3055	O CP	LEU A		22.865	24.900	72.532	1.00 29.25
15	15	ATOM		CB	LEU A		19.841	26.300	72.937	1.00 19.24
	13		3056	CG	LEU A		19.427	24.868	72.632	1.00 17.17
		ATOM	3057		LEU A		19.717	24.017	73.844	1.00 14.63
		ATOM ATOM	3058		LEU A		17.943	24.808	72.328	1.00 10.16
			3059	N	LEU A		22.217	26.659	71.262	1.00 24.49
	20	ATOM	3060	CA	LEU A		23.050	26.340	70.107	1.00 25.05
	20	ATOM	3061	C	LEU A		24.531	26.256	70.383	1.00 32.31
20		ATOM	3062	0	LEU A		25.183	25.301	69.932	1.00 33.60
		ATOM	3063	CB	LEU A		22.765	27.152	68.844	1.00 23.33
		ATOM	3064	CG	LEU A		21.307	27.026	68.442	1.00 23.38
	25	ATOM	3065		LEU A		20.986	28.025	67.334	1.00 20.84
	23	ATOM	3066		LEU A		20.988	25.591	68.017	1.00 18.86
		ATOM	3067	N	PHE A		25.058	27.231	71.127	1.00 28.52
		ATOM	3068	CA	PHE A		26.480	27.236	71.494	1.00 27.82
25		ATOM	3069	С	PHE A		26.813	25.992	72.312	1.00 28.67
	30	ATOM	3070	0	PHE A		27.839	25.331	72.148	1.00 26.96
	30	ATOM	3071	CB	PHE A		26.834	28.455	72.341	1.00 28.60
		ATOM	3072	CG	PHE A		28.296	28.786	72.283	1.00 30.53
		MOTA	3073		PHE A		28.967	28.816	71.064	1.00 35.08
		ATOM	3074		PHE A		29.020	29.063	73.440	1.00 36.52
20	35	ATOM	3075		PHE A		30.320	29.142	70.983	1.00 37.61
30	33	ATOM	3076		PHE A		30.378	29.383	73.382	1.00 40.61
		ATOM	3077	CZ	PHE A		31.026	29.432	72.148	1.00 37.64
		ATOM	3078	N	TYR A		25.913	25.699	73.225	1.00 24.90
		ATOM	3079	CA	TYR A		26.044	24.550	74.065	1.00 24.66
	40	ATOM	3080	C	TYR A		26.106	23.298	73.186	1.00 34.30
	40	ATOM	3081	0	TYR A		27.058	22.558	73.268	1.00 37.51
35		ATOM	3082	CB	TYR A		24.821	24.501	74.967	1.00 26.39
		ATOM	3083	CG	TYR A		24.631	23.181	75.678	1.00 31.99
		ATOM	3084		TYR A		25.546	22.715	76.625	1.00 35.17
	45	MOTA	3085		TYR A		23.501	22.397	75.432	1.00 32.49
	45	ATOM	3086		TYR A		25.341	21.512	77.306	1.00 39.01
		ATOM	3087	CE2			23.281	21.184	76.094	1.00 31.50
		ATOM ATOM	3088 3089	CZ	TYR A		24.206	20.743	77.035	1.00 34.08
40				ОН	TYR A		23.986	19.564	77.683	1.00 36.46
	50	ATOM ATOM	3090 3091	N	LEU A		25.101	23.067	72.310	1.00 31.02
	50	ATOM	3091	CA			25.043	21.889	71.410	1.00 29.65
				C	LEU A		26.274	21.616	70.507	1.00 32.03
		ATOM	3093	0	LEU A		26.664	20.468	70.267	1.00 27.90
		ATOM	3094	CB	LEU A		23.758	21.905	70.552	1.00 28.85
	55	ATOM	3095	CG	LEU A		22.489	21.688	71.375	1.00 30.33
45	"	ATOM	3096		LEU A		21.256	22.047	70.559	1.00 27.38
		ATOM	3097		LEU A		22.400	20.246	71.865	1.00 29.76
		ATOM	3098	N	GLU A		26.841	22.701	69.980	1.00 30.84
		ATOM	3099	CA	GLU A		28.000	22.727	69.118	1.00 30.05
	60	ATOM	3100	C	GLU A		29.210	22.214	69.868	1.00 39.16
	UU	ATOM	3101	0	GLU A		30.089	21.595	69.299	1.00 42.14
50		ATOM	3102	CB	GLU A		28.300	24.204	68.756	1.00 31.03
50		ATOM	3103	CG	GLU A		29.776	24.406	68.376	1.00 37.11
		ATOM	3104	CD OF1	GLU A		30.182	25.830	68.208	1.00 45.20
		ATOM	3105	OEI	GLU A	394	29.614	26.609	67.471	1.00 56.77

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5		ATOM	3106	OE:	2 GLU A 394	31.229	26.133	68.927	1 00 20 77
		ATOM	3107		GLN A 395		22.534	71.160	1.00 39.77
		ATOM	3108	CA	GLN A 395		22.139	72.029	
		MOTA	3109		GLN A 395	30.143	20.690	72.435	1.00 32.86
	5	ATOM	.3110		GLN A 395		19.899		1.00 38.65
		MOTA	3111		GLN A 395		23.051	72.507	1.00 38.67
		ATOM	3112		GLN A 395	30.831		73.287	1.00 33.17
10		ATOM	3113		GLN A 395		24.540	72.996	1.00 13.79
,•		ATOM	3114		GLN A 395	31.176	25.354	74.247	1.00 37.45
	10	ATOM	3115	MES	CLN A 395	30.909	24.959	75.407	1.00 26.89
	10	ATOM					26.523	74.010	1.00 31.99
			3116		LEU A 396		20.352	72.682	1.00 38.68
		ATOM	3117	CA	LEU A 396		19.015	73.083	1.00 38.49
		ATOM	3118	C	LEU A 396	28:633	18.017	71.924	1.00 39.28
45	1.5	ATOM	3119	0	LEU A 396	29.012	16.871	72.100	1.00 42.17
15	15	ATOM	3120	СВ	LEU A 396	27.055	19.072	73.628	1.00 37.93
		ATOM	3121	ÇG	LEU A 396	26.389	17.732	73.946	1.00 42.72
		MOTA	3122		LEU A 396	26.436	17.489	75.445	1.00 45.42
		ATOM	3123	CD2	LEU A 396	24.917	17.709	73.527	1.00 43.42
		ATOM	3124	N	LEU A 397	28.303	18.456	70.730	
	20	ATOM	3125	CA	LEU A 397	28.337	_		1.00 28.48
		ATOM	3126	c	LEU A 397	29.620	17.595	69.589	1.00 25.49
20		ATOM	3127	ŏ			17.609	68.771	1.00 36.86
		ATOM	3128		LEU A 397	29.596	17.220	67.599	1.00 39.85
		ATOM		CB	LEU A 397	27.156	17.924	68.686	1.00 23.73
	25		3129	CG	LEU A 397	25.843	17.773	69.401	1.00 25.82
	23	ATOM	3130		LEU A 397	24.740	18.559	68.669	1.00 22.99
		MOTA	3131		LEU A 397	25.525	16.272	69.452	1.00 27.30
		ATOM	3132	N	GLY A 398	30.731	18.069	69.342	1.00 33.98
25		ATOM	3133	CA	GLY A 398	31.993	18.038	68.617	1.00 34.14
	00	ATOM	3134	С	GLY A 398	32.547	19.260	67.889	1.00 38.92
	30	ATOM	3135	0	GLY A 398	33.502	19.097	67.115	1.00 39.98
		ATOM	3136	N	GLY A 399	32.001	20.457	68.105	1.00 33.96
		ATOM	3137	CA	GLY A 399	32.543	21.650	67.440	
		ATOM	3138	С	GLY A 399	31.713	22.336		1.00 30.35
		ATOM	3139	Ō	GLY A 399	30.800		66.365	1.00 31.72
30	35	ATOM	3140	N	PRO A 400		21.823	65.762	1.00 34.57
30		ATOM	3141	CA		32.076	23.550	66.124	1.00 33.01
		ATOM	3142		PRO A 400	31.429	24.406	65.151	1.00 35.02
		ATOM	3143	C	PRO A 400	31.379	23.794	63.750	1.00 43.93
				0	PRO A 400	30.360	23.838	63.045	1.00 40.14
	40	ATOM	3144	СВ	PRO A 400	32.293	25.672	65.111	1.00 35.73
	40	ATOM	3145	CG	PRO A 400	33.539	25.411	65.948	1.00 38.03
		ATOM	3146	CD	PRO A 400	33.423	24.010	66.517	1.00 33.92
35		ATOM	3147	N	GLU A 401	32.512	23.237	63.345	1.00 43.85
		MOTA	3148	CA	GLU A 401	32.597	22.620	62.042	1.00 42.92
	4.5	ATOM	3149	С	GLU A 401	31.491	21.587	61.878	1.00 37.92
	45	ATOM	3150	0	GLU A 401	30.810	21.588	60.866	1.00 37.32
		ATOM	3151	CB	GLU A 401	33.996	22.034	61,789	
		ATOM	3152	CG	GLU A 401	34.578	22.372		1.00 45.93
		ATOM	3153	CD	GLU A 401	35.603		60.398	1.00 69.62
40		ATOM	3154		GLU A 401		21.373	59.911	1.00100.00
	50	ATOM	3155	OE2	GLU A 401	36.702	21.236	60.427	1.00100.00
		ATOM	3156	N		35.195	20.689	58.865	1.00 93.16
		ATOM			ILE A 402	31.317	20.720	62.902	1.00 34.58
			3157	CA	ILE A 402	30.281	19.681	62.922	1.00 33.20
		ATOM	3158	С	ILE A 402	28.898	20.291	62.938	1.00 39.09
	66	ATOM	3159	0	ILE A 402	28.065	19.896	62.133	1.00 41.43
45	55	ATOM	3160	CB	ILE A 402	30.391	18.673	64.078	1.00 33.82
,,,		ATOM	3161	CG1	ILE A 402	31.490	17.661	63.811	1.00 34.70
		ATOM	3162	CG2	ILE A 402	29.080	17.900	64.287	
		ATOM	3163		ILE A 402	31.878	16.896	65.080	1.00 23.32
		ATOM	3164	N	PHE A 403	28.668	21.246		1.00 49.20
	60	ATOM	3165	CA	PHE A 403	27.390		63.868	1.00 32.73
		ATOM	3166	C	PHE A 403		21.952	64.044	1.00 29.52
50		ATOM	3167	Ö	PHE A 403	27.032	22.816	62.836	1.00 33.94
50		ATOM	3168			25.866	23.022	62.469	1.00 34.15
		ATOM		CB	PHE A 403	27.319	22.719	65.381	1.00 29.03
		ATOM	3169	CG	PHE A 403	25.917	22.783	65.929	1.00 28.54

5		MOTA	3170	CD1	PHE A	403	25.323	21.643	66.484	1.00	29.91
		ATOM	3171	CD2	PHE A	403	25.176	23.964	65.873		27.62
		MOTA	3172		PHE A		24.021	21.667	66.990		27.38
	_	MOTA	3173	CE2	PHE A	403	23.881	24.017	66.393		28.82
	5	MOTA	3174	CZ	PHE A		23.304	22.863	66.932		25.72
		ATOM	3175	N	LEU A		28.040	23.327	62.165	1.00	31.31
10		ATOM	3176	CA	LEU A		27.687	24.080	60.983	1.00	32.95
10		ATOM	3177	С	LEU A		27.068	23.099	59.952	1.00	32.89
	10	MOTA	3178	0	LEU A		26.050	23.361	59.315	1.00	37.36
	10	ATOM	3179	CB	LEU A		28.798	25.045	60.464		33.15
		MOTA	3180	CG	LEU A		29.029	26.208	61.444		36.96
		atom Atom	3181 3182		LEU A		30.454	26.717	61.353		37.13
		ATOM	3183	N	LEU A		28.083	27.362	61.163		39.27
15	15	ATOM	3184	CA	GLY A GLY A		27.670 27.167	21.921	59.826		22.02
	15	ATOM	3185	C	GLY A			20.908	58.928		22.77
		ATOM	3186	ŏ	GLY A		25.698 24.885	20.676	59.206		31.85
		ATOM	3187	N	PHE A		25.364	20.438 20.747	58.297		33.01
		ATOM	3188	CA	PHE A		23.992	20.747	60.493		26.28
	20	ATOM	3189	Ç.	PHE A		23.188	21.757	60.863 60.365		25.27
		ATOM	3190	ō	PHE A		22.195	21.629	59.638		34.80
20 .		ATOM	3191	СВ	PHE A		23.798	20.268	62.351		36.22
		ATOM	3192	CG	PHE A		22.388	20.525	62.798		24.52
		ATOM	3193		PHE A		21.328	19.734	62.353		28.50
	25	ATOM	3194		PHE A		22.107	21.579	63.669		30.12
		ATOM	3195		PHE A		20.025	19.977	62.793		31.40
		ATOM	3196		PHE A		20.810	21.862	64.105		32.57
25		ATOM	3197	CZ	PHE A		19.771	21.037	63.669		31.88
		ATOM	3198	N	LEU A		23.661	22.934	60.708		32.11
	30	ATOM	3199	CA	LEU A		22.972	24.132	60.269		33.11
		ATOM	3200	С	LEU A	407	22.706	24.204	58.767		34.74
		ATOM	3201	0	LEU A	407	21.635	24.615	58.341		35.21
		ATOM	3202	СВ	LEU A	407	23.589	25.420	60.840		35.36
		ATOM	3203	CG	LEU A	407	22.597	26.577	60.855		41.79
30	35	ATOM	3204		LEU A		23.048	27.626	61.833		40.45
		ATOM	3205	CD2	LEU A	407	22.513	27.197	59.461		49.57
		ATOM	3206	N .	LYS A	408	23.667	23.804	57.948		34.92
		ATOM	3207	CA	LYS A		23.476	23.826	56.490	1.00	36.29
	40	ATOM	3208	С	LYS A		22.378	22.876	56.037	1.00	38.15
	40	ATOM	3209	0	LYS A		21.568	23.191	55.160	1.00	35.09
35		ATOM	3210	CB	LYS A		24.747	23.517	55.707	1.00	40.54
30		ATOM	3211	CG	LYS A		24.633	23.873	54.214	1.00	43.41
		ATOM	3212	CD	LYS A		25.950	23.796	53.422	1.00	49.26
	45	ATOM	3213	CE	LYS A		26.808	25.059	53.459	1.00	61.45
	40	ATOM ATOM	3214	NZ	LYS A		28.014	24.994	52.606		73.78
		ATOM	3215 3216	N	ALA A		22.352	21.690	56.655		35.34
		ATOM	3217	CA	ALA A		21.333	20.698	56.298		36.14
40		ATOM	3218	С 0	ALA A		19.927	21.041	56.814		38.45
	50	ATOM	3219	СВ	ALA A		18.913	20.821	56.134		37.39
	20	ATOM	3220	N	TYR A		21.762	19.273	56.626		36.66
		ATOM	3221	CA	TYR A		19.902 18.693	21.597	58.030		33.14
		ATOM	3222	C	TYR A		18.028	22.059	58.682		29.65
		ATOM	3223	ō	TYR A		16.855	23.051	57.730		35.55
45	55	ATOM	3224	СВ	TYR A		19.117	22.976	57.399		37.26
45		ATOM	3225	CG	TYR A		18.069	22.762	59.970		24.67
		ATOM	3226		TYR A		16.861	23.643	60.541		26.95
		ATOM	3227		TYR A		18.288		60.990		28.10
		ATOM	3228		TYR A		15.883	25.015 23.924	60.663		29.66
	60	ATOM	3229		TYR A		17.316	25.839	61.571		26.98
		ATOM	3230	CZ	TYR A		16.112	25.294	61.230 61.685		31.84
50		ATOM	3231	ОН	TYR A		15.156	26.110	62.241		37.49
		ATOM	3232	N	VAL A		18.848	23.961	57.262		33.48
		ATOM	3233	CA	VAL A		18.457	24.984	56.341		28.75
							_3.137	-3.707	20.211	1.00	29.23

5		ATOM	3234	. с	VAL A	411	18.013	24.469	54.992	1.00 34.00
		ATOM	3235	0	VAL A		17.060	24.982	54.401	1.00 30.00
		MOTA	3236	CB	VAL A		19.617	25.922	56.139	1.00 32.22
	_	ATOM	3237	CG1	VAL A	411	19.331	26.821	54.950	1.00 29.86
	5	ATOM	3238	CG2	VAL A	411	19.850	26.708	57.431	1.00 31.69
		ATOM	3239	N	GLU A	412	18.730	23.479	54.488	1.00 33.14
40		ATOM	3240	CA	GLU A	412	18.402	22.900	53.217	1.00 31.91
10		MOTA	3241	С	GLU A	412	17.068	22.163	53.355	1.00 30.32
	••	MOTA	3242	0	GLU A	412	16.182	22.225	52.531	1.00 31.89
	10	ATOM	3243	CB	GLU A	412	19.502	21.883	52.932	1.00 36.48
		ATOM	3244	CG	GLU A		20.443	22.174	51.737	1.00 67.01
		ATOM	3245	CD	GLU A		21.872	21.699	51.962	1.00100.00
		ATOM	3246		GLU A		22.193	20.782	52.716	1,00100,00
15	15	ATOM	3247		GLU A		22.750	22.396	51.277	1.00 94.73
,,,	15	ATOM	3248	N	LYS A		16.922	21.444	54.444	1.00 22.18
		ATOM	3249	CA	LYS A		15.729	20.692	54.714	1.00 17.91
		ATOM	3250	C	LYS A		14.463	21.486	54.855	1.00 23.75
		ATOM	3251	0	LYS A		13.417	20.978	54.503	1.00 25.92
	20	ATOM	3252	CB	LYS A		15.890	19.911	55.988	1.00 15.65
	20	ATOM	3253 3254	CG	LYS A		14.554	19.422	56.503	1.00 38.69
20		MOTA MOTA	3255	CD	LYS A		14.150	18.089	55.903	1.00 58.11
		ATOM	3256	CE NZ	LYS A LYS A		13.634	17.099	56.937	1.00 64.98
		ATOM	3257	N	PHE A		13.457	15.751	56.381	1.00 73.89
	25	ATOM	3258	CA	PHE A		14.530 13.316	22.688 23.479	55.424	1.00 25.40
		ATOM	3259	c	PHE A		13.151	24.748	55.640	1.00 27.80
		ATOM	3260	ō	PHE A		12.276	25.557	54.821 55.122	1.00 35.82 1.00 35.17
25		ATOM	3261	СВ	PHE A		13.063	23.791	57.118	1.00 30.46
25		ATOM	3262	CG	PHE A		12.936	22.553	57.964	1.00 33.88
	30	ATOM	3263		PHE A		11.746	21.826	57.996	1.00 35.94
		ATOM	3264		PHE A		14.005	22.110	58.742	1.00 37.75
		ATOM	3265		PHE A		11.629	20.664	58.761	1.00 37.77
		ATOM	3266	CE2	PHE A	414	13.888	20.962	59.526	1.00 42.23
		ATOM	3267	CZ	PHE A	414	12.698	20.231	59.542	1.00 39.10
30	35	ATOM	3268	N	SER A	415	13.970	24.933	53.795	1.00 36.12
		MOTA	3269	CA	SER A	415	13.858	26.115	52.945	1.00 36.36
		ATOM	3270	С	SER A	415	12.412	26.295	52.510	1.00 38.99
		ATOM	3271	0	SER A	415	11.730	25.315	52.243	1.00 41.04
	40	ATOM	3272	CB	SER A		14.773	26.008	51.736	1.00 37.43
	40	ATOM	3273	OG	SER A		16.036	26,566	52.046	1.00 46.73
35		ATOM	3274	N	TYR A		11.928	27.537	52.475	1.00 33.40
55		ATOM	3275	CA	TYR A		10.541	27.832	52.072	1.00 30.88
		ATOM	3276	C	TYR A		9.453	27.183	52.947	1.00 33.62
	45	ATOM ATOM	3277 3278	O	TYR A		8.295	27.095	52.546	1.00 33.44
	72	ATOM	3279	CB CG	TYR A		10.292	27.479	50.584	1.00 28.42
		ATOM	3280		TYR A TYR A		11.496	27.782	49.723	1.00 24.76
		ATOM	3281		TYR A		11.791 12.375	29.087	49.338	1.00 26.55
40		ATOM	3282	CFI	TYR A	116	12.914	26.778 29.384	49.335	1.00 21.68
	50	ATOM	3283		TYR A		13.504	27.052	48.570 48.572	1.00 25.16
	•••	ATOM	3284	CZ			13.780	28.360	48.189	1.00 20.15
		ATOM	3285	ОН	TYR A		14.892	28.616	47.399	1.00 35.15
		ATOM	3286	N	LYS A		9.823	26.713	54.122	1.00 27.67
		ATOM	3287	CA	LYS A		8.889	26.065	55.008	1.00 28.02
45	55	ATOM	3288	C	LYS A		8.733	26.830	56.317	1.00 31.36
40		ATOM	3289	0	LYS A		9.547	27.671	56.682	1.00 33.15
		ATOM	3290	СВ	LYS A		9.335	24.615	55.252	1.00 33.86
		ATOM	3291	CG	LYS A		8.449	23.792	56.201	1.00 86.28
		ATOM	3292	CD	LYS A		8.742	22.275	56.232	1.00100.00
	60	ATOM	3293	CE	LYS A		7.924	21.471	57.265	1.00 72.28
		ATOM	3294	NZ	LYS A		8.280	20.033	57.323	1.00 41.88
50		MOTA	3295	N	SER A		7.668	26.557	57.033	1.00 28.88
		ATOM	3296	CA	SER A		7.455	27.195	58.335	1.00 30.04
		ATOM	3297	С	SER A		7.425	26.064	59.332	1.00 34.09

5		ATOM	3298	0	SER A	418	6.614	25.145	59.193	1.00 31.54
		ATOM	3299	CB	SER A	418	6.261	28.126	58.410	1.00 31.46
		ATOM	3300	OG	SER A		6.417	29.106	57.399	1.00 35.01
		ATOM	3301	N	ILE A	419	8.356	26.077	60.281	1.00 28.50
	5	ATOM	3302	CA	ILE A		8.446	24.971	61.205	1.00 23.86
		ATOM	3303	С	ILE A		8.272	25.342	62.641	1.00 25.06
		ATOM	3304	ō	ILE A		8.122	26.500	63.002	1.00 21.64
10		ATOM	3305	СВ	ILE A		9.803	24.314	61.026	1.00 25.02
		ATOM	3306		ILE A		10.863	25.325	61.399	1.00 23.62
	10	ATOM	3307		ILE A		10.051	23.937	59.565	1.00 23.22
		ATOM	3308		ILE A		12.236	24.688	61.253	1.00 23.22
		ATOM	3309	N	THR A		8.321	24.302	63.455	
		ATOM	3310	CA	THR A		8.201	24.417		1.00 24.71 1.00 24.36
		ATOM	3311	C	THR A		9.416	23.795	64.895 65.538	
15	15	ATOM	3312	õ	THR A		10.190			1.00 28.90
	13	ATOM	3312					23.112	64.863	1.00 23.38
			3313	CB OC1	THR A		6.979	23.691	65.448	1.00 24.92
		ATOM			THR A		7.190	22.313	65.291	1.00 26.43
		ATOM	3315		THR A		5.728	24.082	64.694	1.00 31.57
	20	ATOM	3316	N	THR A		9.542	24.051	66.855	1.00 29.30
	20	ATOM	3317	CA	THR A		10.610	23.549	67.709	1.00 27.78
20		ATOM	3318	C	THR A		10.831	22.035	67.585	1.00 30.99
		ATOM	3319	0	THR A		11.975	21.594	67.489	1.00 33.28
		ATOM	3320	СВ	THR A		10.394	23.969	69.166	1.00 21.94
	~ ~	MOTA	3321		THR A		10.567	25.369	69.263	1.00 24.52
	25	ATOM	3322	CG2	THR A	421	11.399	23.221	70.045	1.00 20.12
		ATOM	3323	N	ASP A	422	9.721	21.272	67.575	1.00 21.94
		ATOM	3324	CA	ASP A	422	9.706	19.823	67.430	1.00 21.08
25		ATOM	3325	C	ASP A	422	10.323	19.401	66.104	1.00 31.16
		ATOM	3326	0	ASP A	422	11.110	18.427	66.027	1.00 31.95
	30	ATOM	3327	CB	ASP A	422	8.276	19.278	67.561	1.00 19.49
		ATOM	3328	CG	ASP A		8.236	17.802	67.298	1.00 31.85
		ATOM	3329	OD1	ASP A		9.130	17.040	67.654	1.00 29.73
		ATOM	3330		ASP A		7.197	17.415	66.598	1.00 56.60
		ATOM	3331	N	ASP A		9.957	20.146	65.049	1.00 26.75
30	35	ATOM	3332	CA	ASP A		10.505	19.876	63.729	1.00 26.01
		ATOM	3333	ç.	ASP A		12.027	19.957	63.830	1.00 40.09
		ATOM	3334	ō	ASP A		12.753	19.020	63.500	1.00 47.09
		ATOM	3335	ĊВ	ASP A		10.000	20.833	62.631	1.00 24.86
		ATOM	3336	CG	ASP A		8.538	20.722	62.343	1.00 39.90
	40	ATOM	3337		ASP A		7.968			
	70	ATOM	3338		ASP A		7.943	19.649	62.299	1.00 45.03
35		ATOM	3339	N N				21.887	62.113	1.00 40.43
		ATOM	3340	CA	TRP A		12.493	21.099	64.320	1.00 31.92
		ATOM	3341		TRP A		13.903	21.372	64.495	1.00 29.69
	45			C	TRP A		14.611	20.271	65.282	1.00 33.81
	73	MOTA	3342	0	TRP A		15.537	19.616	64.824	1.00 35.87
		ATOM	3343	CB	TRP A		14.056	22.711	65.239	1.00 26.11
		ATOM	3344	CG	TRP A		15.431	22.869	65.786	1.00 27.05
40		ATOM	3345		TRP A		16.518	23.302	65.101	1.00 29.65
	50	ATOM	3346		TRP A		15.885	22.587	67.119	1.00 26.62
	50	ATOM	3347		TRP A		17.612	23.321	65.922	1.00 27.83
		ATOM	3348		TRP A		17.257		67.163	1.00 28.62
		ATOM	3349		TRP A		15.260	22.138	68.269	1.00 29.69
		ATOM	3350		TRP A		18.010	22.758	68.319	1.00 29.28
		ATOM	3351		TRP A		16.000	21.993	69.429	1.00 33.50
45	55	MOTA	3352	CH2	TRP A	424	17.362	22.317	69.459	1.00 33.93
		ATOM	3353	N	LYS A	425	14.156	20.090	66.497	1.00 28.75
		ATOM	3354	CA	LYS A		14.723	19.105	67.373	1.00 29.43
		ATOM	3355	С	LYS A		14.697	17.691	66.808	1.00 29.49
		ATOM	3356	Ó	LYS A		15.627	16.928	67.030	1.00 27.65
	60	ATOM	3357	СВ	LYS A		14.078	19.171	68.744	1.00 29.70
•		ATOM	3358	CG	LYS A		14.860	18.414	69.787	1.00 28.11
50		ATOM	3359	CD	LYS A		14.161	18.409	71.132	1.00 23.57
		ATOM	3360	CE	LYS A		14.300	17.063	71.132	1.00 23.37
		ATOM	3361	NZ	LYS A		13.042		71.768	
		AION	2301	14.7	ьтэ А	423	13.042	16.302	11.108	1.00 58.08

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5		ATOM	3362	N.	ASP A		13.606	17.361	66.107	1.00 19.05
		ATOM	3363	CA	ASP A	426	13.417	16.070	65.516	1.00 18.43
		ATOM	3364	С	ASP A	426	14.453	15.879	64.387	1.00 28.33
		ATOM	3365	0	ASP A	426	15.070	14.832	64.232	1.00 31.25
	5	ATOM	3366	CB	ASP A		11.920	15.840	65.098	1.00 19.79
		MOTA	3367	CG	ASP A		10.998	15.575	66.274	1.00 25.54
40		MOTA	3368		ASP A		11.341	15.466	67.409	1.00 29.73
10		ATOM	3369	OD2	ASP A		9.804	15.611	65.938	1.00 20.67
		ATOM	3370	N	PHE A	427	14.674	16.926	63.612	1.00 25.09
	10	MOTA	3371	CA	PHE A	427	15.654	16.899	62.540	1.00 25.81
		ATOM	3372	С	PHE A	427	17.066	16.718	63.159	1.00 34.01
		ATOM	3373	0	PHE A	427	17.843	15.851	62.773	1.00 36.25
		ATOM	3374	CB	PHE A	427	15.589	18.197	61.704	1.00 26.35
15		ATOM	3375	CG	PHE A	427	16.698	18.202	60.702	1.00 27.40
15	15	ATOM	3376	CD1	PHE A	427	16.714	17.247	59.686	1.00 29.97
		MOTA	3377	CD2	PHE A	427	17.773	19.084	60.805	1.00 28.71
		ATOM	3378	CE1	PHE A	427	17.730	17.194	58.733	1.00 27.72
		ATOM	3379	CE2	PHE A	427	18.806	19.046	59.867	1.00 30.37
		ATOM	3380	CZ	PHE A	427	18.780	18.104	58.837	1.00 26.34
	20	ATOM	3381	N	LEU A	428	17.369	17.544	64.160	1.00 28.94
20		ATOM	3382	CA	LEU A	428	18.622	17.496	64.924	1.00 27.74
20		ATOM	3383	C	LEU A	428	18.989	16.047	65.303	1.00 32.08
		ATOM	3384	0	LEU A	428	20.145	15.647	65.209	1.00 36.38
		ATOM	3385	CB	LEU A		18.510	18.362	66.223	1.00 24.68
	25	ATOM	3386	CG	LEU A		19.778	18.377	67.079	1.00 24.30
		ATOM	3387		LEU A		20.855	19.278	66.467	1.00 23.00
		ATOM	3388		LEU A		19.446	18.856	68.481	1.00 16.41
25		ATOM	3389	N	TYR A		17.991	15.271	65.735	1.00 23.71
		ATOM	3390	CA	TYR A		18.148	13.896	66.144	1.00 23.18
	30	ATOM	3391	С	TYR A		18.311	12.967	64.976	1.00 26.62
		ATOM	3392	ō	TYR A		18.911	11.910	65.076	1.00 28.43
		ATOM	3393	СВ	TYR A		16.921	13.453	66.914	1.00 25.59
		ATOM	3394	CG	TYR A		17.069	13.526	68.414	1.00 29.53
		ATOM	3395		TYR A		16.823	14.714	69.114	1.00 23.33
30	35	ATOM	3396		TYR A		17.361	12.383	69.156	1.00 32.70
		ATOM	3397		TYR A		16.916	14.769	70.510	1.00 32.70
		ATOM	3398	CE2	TYR A		17.485	12.420	70.551	1.00 35.30
		ATOM	3399	CZ	TYR A		17.251	13.623	71.231	1.00 41.02
		ATOM	3400	ОН	TYR A		17.339	13.679	72.609	1.00 30.02
	40	ATOM	3401	N	SER A		17.748	13.342	63.854	1.00 30.02
		ATOM	3402	CA	SER A		17.914	12.469	62.730	1.00 23.42
35		ATOM	3403	c	SER A		19.264	12.722	62.050	1.00 23.42
		ATOM	3404	ō	SER A		19.879	11.819	61.467	1.00 35.11
		ATOM	3405	СВ	SER A		16.756	12.541	61.773	
	45	ATOM	3406	OG	SER A		17.089	13.475	60.777	1.00 28.79 1.00 49.56
		ATOM	3407	N	TYR A		19.748	13.955	62.132	
		ATOM	3408	CA	TYR A		21.017	14.296	61.537	1.00 27.18
40		ATOM	3409	ç.	TYR A		22.152	13.702	62.316	1.00 27.14
40		ATOM	3410	ŏ	TYR A		23.155	13.702		1.00 32.52
	50	ATOM	3411	СВ	TYR A		21.216	15.818	61.771	1.00 33.64
		ATOM	3412	CG	TYR A		22.566		61.385	1.00 31.07
		ATOM	3413		TYR A			16.265	60.812	1.00 35.63
		ATOM	3414		TYR A		23.663 22.735	16.492	61.650	1.00 36.88
		ATOM	3415		TYR A		24.894	16.496	59.444	1.00 36.92
45	55	ATOM	3416		TYR A			16.924	61.157	1.00 33.78
45	33	ATOM	3417				23.964	16.916	58.924	1.00 37.86
				CZ	TYR A		25.038	17.143	59.786	1.00 46.01
		ATOM	3418	OH	TYR A		26.247	17.573	59.294	1.00 51.28
		ATOM	3419	И	PHE A		21.964	13.728	63.606	1.00 29.66
	60	ATOM	3420	CA	PHE A		22.939	13.215	64.526	1.00 29.12
	v	ATOM	3421	C	PHE A		22.522	11.865	65.007	1.00 42.64
50		ATOM	3422	0	PHE A		22.499	11.593	66.197	1.00 46.77
55		ATOM	3423	CB	PHE A		23.063	14.157	65.719	1.00 30.24
		ATOM	3424	CG	PHE A		23.962	15.327	65.401	1.00 33.03
		ATOM	3425	CDI	PHE A	432	25.336	15.113	65.277	1.00 37.22

5		ATOM	3426	CD2	PHE A	432	23.470	16.624	65.232	1.00 30.70
		ATOM	3427	CE1	PHE A	432	26.223	16.153	64.999	1.00 34.27
		MOTA	3428	CE2	PHE A	432	24.349	17.667	64.938	1.00 31.71
		ATOM	3429	CZ	PHE A	432	25.722	17.438	64.823	1.00 27.82
	5	MOTA	3430	N	LYS A	433	22.174	11.029	64.063	1.00 42.50
		MOTA	3431	CA	LYS A		21.669	9.670	64.270	1.00 40.87
		ATOM	3432	C	LYS A		22.718	8.751	64.908	1.00 46.17
10		ATOM	3433	0	LYS A		22.405	7.734	65.513	1.00 48.48
		ATOM	3434	СВ	LYS A		21.245	9.106	62.917	1.00 39.25
	10	ATOM	3435	CG	LYS A		19.988	8.241	63.017	1.00 84.17
		ATOM	3436	CD	LYS A		18.925	8.660	62.000	1.00100.00
		ATOM	3437	CE	LYS A		17.523	8.172	62.384	1.00100.00
		ATOM	3438	ΝZ	LYS A		16.525	9.119	61.884	1.00100.00
		ATOM	3439	N	ASP A		24.002	9.112	64.697	1.00 45.20
15	15	ATOM	3440	CA	ASP A		25.083	8.349	65.321	1.00 47.80
		ATOM	3441	c c	ASP A		25.201	8.684	66.802	
		ATOM	3442	ō	ASP A		25.474	7.845		1.00 50.78
		ATOM	3443	СВ	ASP A		26.405	8.567	67.653	1.00 55.76
		ATOM	3444	CG	ASP A		26.123		64.562	1.00 53.91
	20	ATOM	3445					8.474	63.069	1.00 93.32
	20				ASP A		25.744	7.573	62.325	1.00 96.22
20		ATOM	3446		ASP A		26.119	9.664	62.753	1.00100.00
		ATOM	3447	N	LYS A		25.015	9.978	67.085	1.00 38.82
		ATOM	3448	CA	LYS A		24.974	10.404	68.468	1.00 34.57
	25	ATOM	3449	С	LYS A		23.549	10.749	68.881	1.00 39.87
	25	ATOM	3450	0	LYS A		23.070	11.840	68.693	1.00 40.34
		ATOM	3451	СВ	LYS A		25.864	11.631	68.615	1.00 34.69
		ATOM	3452	CG	LYS A		27.064	11.595	67.679	1.00 40.86
25		ATOM	3453	CD	LYS A		27.703	12.975	67.532	1.00 51.04
		ATOM	3454	CE	LYS A		29.242	12.904	67.557	1.00 24.08
	30	ATOM	3455	NZ	LYS A		29.822	13.990	66.760	1.00 45.26
		ATOM	3456	N	VAL A	436	22.843	9.728	69.414	1.00 38.07
		ATOM	3457	CA	VAL A	436	21.601	10.036	70.111	1.00 36.86
		ATOM	3458	С	VAL A	436	21.846	10.129	71.608	1.00 44.88
	0_	ATOM	3459	0	VAL A	436	21.289	10.948	72.300	1.00 46,42
30	35	ATOM	3460	CB	VAL A	436	20.567	8.923	69.816	1.00 37.37
		ATOM	3461	CG1	VAL A	436	19.944	9.143	68.446	1.00 36.24
		ATOM	3462	CG2	VAL A	436	21.227	7.556	69.854	1.00 36.80
		ATOM	3463	N	ASP A	437	22.718	9.232	72.099	1.00 43.61
	•	ATOM	3464	CA	ASP A	437	23.044	9.222	73.522	1.00 41.43
	40	ATOM	3465	С	ASP A	437	23.657	10.546	73.958	1.00 45.71
		ATOM	3466	0	ASP A		23.554	10.956	75.107	1.00 49.89
35		ATOM	3467	СВ	ASP A		24.022	8.082	73.776	1.00 43.84
		ATOM	3468	CG	ASP A		23.281	6.752	73.691	1.00 72.47
		ATOM	3469		ASP A		22.062	6.769	73.823	1.00 74.64
	45	ATOM	3470		ASP A		23.933	5.730	73.481	1.00 86.09
		ATOM	3471	N	VAL A		24.333	11.324	73.122	1.00 40.21
		ATOM	3472	CA	VAL A		24.807	12.624	73.577	1.00 40.97
40		ATOM	3473	C	VAL A		23.621	13.582	73.668	1.00 41.86
40		ATOM	3474	ō	VAL A		23.368	14.276	74.657	1.00 39.95
	50	ATOM	3475	СВ	VAL A		25.875	13.165	72.615	
	50	ATOM	3476		VAL A		26.438			1.00 47.47
		ATOM	3477				26.996	14.523	73.051	1.00 47.51
		ATOM	3478		VAL A			12.149	72.440	1.00 47.51
		ATOM	3479	N	LEU A		22.876	13.595	72.585	1.00 37.91
4.5	55	ATOM		CA	LEU A		21.729	14.442	72.507	1.00 36.21
45	<i>JJ</i>		3480	C	LEU A		20.850	14.190	73.695	1.00 40.03
		ATOM	3481	0	LEU A		20.214	15.064	74.255	1.00 42.22
		ATOM	3482	CB	LEU A		20.949	14.180	71.210	1.00 33.84
		ATOM	3483	CG	LEU A		21.552	14.939	70.039	1.00 32.80
	C O	ATOM	3484		LEU A		20.813	14.538	68.775	1.00 34.08
	60	ATOM	3485		LEU A		21.435	16.434	70.258	1.00 23.80
50		ATOM	3486	N	ASN A		20.810	12.953	74.076	1.00 34.03
50		ATOM	3487	CA	asn a		19.971	12.603	75.187	1.00 34.00
		ATOM	3488	С	ASN A	440	20.494	13.093	76.532	1.00 40.95
		ATOM	3489	0	ASN A	440	19.816	12.995	77.544	1.00 42.09

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5		MOTA	3490	СB	ASN A		19.681	11.095	75.178	1.00 24.89
		ATOM	3491	CG	asn a		18.790	10.635	74.028	1.00 46.52
		MOTA	3492	OD1	ASN A	440	19.005	9.537	73.480	1.00 58.82
	_	ATOM	3493	ND2	ASN A	440	17.769	11.440	73.680	1.00 31.11
	5	ATOM	3494	N	GLN A	441	21.707	13.623	76.531	1.00 36.98
		ATOM	3495	CA	GLN A	441	22.339	14.095	77.744	1.00 35.47
		ATOM	3496	С	GLN A	441	21.879	15.478	78.067	1.00 36.00
10		ATOM	3497	0	GLN A	441	22.137	16.029	79.142	1.00 34.96
		ATOM	3498	СВ	GLN A		23.878	14.109	77.581	1.00 38.10
	10	MOTA	3499	CG	GLN A		24.504	12.692	77.422	1.00 52.06
		ATOM	3500	CD	GLN A		25.954	12.730	76.955	1.00 81.69
		ATOM	3501		GLN A		26.476	13.796	76.609	1.00 74.46
		ATOM	3502	NE2			26.616	11.574	76.972	1.00 91.09
		ATOM	3503	N	VAL A		21.197	16.067	77.112	1.00 31.86
15	15	ATOM	3504	CA	VAL A		20.753	17.411	77.384	
	10	ATOM	3505	C	VAL A		19.354			1.00 32.78
		ATOM	3506	Ö				17.468	77.970	1.00 38.24
		ATOM			VALA		18.468	16.700	77.588	1.00 42.83
			3507	CB	VAL A		20.845	18.277	76.159	1.00 34.84
	20	ATOM	3508		VAL A		21.430	17.435	75.020	1.00 34.65
	20	ATOM	3509		VAL A		19.441	18.705	75.811	1.00 33.21
20		ATOM	3510	N	ASP A		19.172	18.388	78.908	1.00 25.60
		ATOM	3511	CA	ASP A		17.931	18.634	79.616	1.00 24.57
		ATOM	3512	С	ASP A		16.996	19.533	78.791	1.00 32.14
	25	MOTA	3513	0	ASP A		16.744	20.732	79.073	1.00 34.77
	25	ATOM	3514	СВ	ASP A		18.332	19.272	80.957	1.00 27.11
		ATOM	3515	CG	ASP A		17.216	19.413	81.901	1.00 39.99
		MOTA	3516		ASP A		16.063	19.234	81.573	1.00 44.78
25		MOTA	3517		ASP A		17.631	19.753	83.094	1.00 56.66
	20	MOTA	3518	N	TRP A		16.525	18.914	77.722	1.00 28.30
	30	MOTA	3519	CA	TRP A		15.614	19.507	76.757	1.00 26.27
		ATOM	3520	С	TRP A	444	14.460	20.296	77.416	1.00 31.52
•		MOTA	3521	0	TRP A	444	14.102	21.409	76.988	1.00 34.63
		ATOM	3522	CB	TRP A	444	15.067	18.398	75.799	1.00 21.47
		ATOM	3523	CG	TRP A	444	16.095	17.951	74.806	1.00 22.03
30	35	ATOM	3524	CD1	TRP A	444	16.675	16.718	74.736	1.00 25.16
		ATOM	3525	CD2	TRP A	444	16.733	18.738	73.776	1.00 20.36
		ATOM	3526	NE1	TRP A	444	17.623	16.677	73.738	1.00 23.97
		ATOM	3527	CE2	TRP A	444	17.688	17.906	73.138	1.00 24.71
		ATOM	3528	CE3	TRP A	444	16.596	20.045	73.342	1.00 20.86
	40	ATOM	3529	CZ2	TRP A	444	18.448	18.345	72.060	1.00 24.51
		ATOM	3530	CZ3	TRP A	444	17.353	20.471	72.264	1.00 22.88
35		ATOM	3531		TRP A		18.281	19.643	71.643	1.00 23.48
		ATOM	3532	N	ASN A		13.855	19.711	78.457	1.00 24.92
		ATOM	3533	CA	ASN A		12.723	20.326	79.113	1.00 26.30
	45	MOTA	3534	С	ASN A		13.040	21.677	79.729	1.00 30.17
		ATOM	3535	0	ASN A		12.291	22.660	79.547	1.00 31.86
		MOTA	3536	СВ	ASN A		11.987	19.382	80.094	1.00 40.83
		ATOM	3537	CG	ASN A		10.946	20.033	81.020	1.00 87.07
40		MOTA	3538		ASN A		11.271	20.635	82.065	1.00 86.38
	50	ATOM	3539		ASN A		9.670	19.848	80.688	1.00 71.65
		ATOM	3540	N	ALA A		14.147	21.687	80.436	1.00 22.70
		ATOM	3541	CA	ALA A		14.583	22.886	81.073	1.00 24.45
		ATOM	3542	c	ALA A		14.886	23.896	79.990	1.00 30.52
		ATOM	3543	ō	ALA A		14.324	25.001	79.936	1.00 30.32
45	55	ATOM	3544	СВ	ALA A		15.814	22.543	81.900	
45	-	ATOM	3545	N	TRP A		15.776			1.00 25.68
		ATOM	3546	CA	TRP A		16.162	23.494	79.102	1.00 25.24
		ATOM	3547	C	TRP A		14.989	24.384	78.034	1.00 26.83
		ATOM	3548	0	TRP A		14.989	24.912 26.089	77.223	1.00 31.32
	60	ATOM	3549	CB	TRP A				76.875	1.00 30.48
	55	ATOM	3550	CG	TRP A		17.166	23.725	77.062	1.00 25.78
50		ATOM	3551		TRP A		18.625	23.815	77.421	1.00 26.60
55		ATOM	3552				19.343	22.840	78.046	1.00 28.89
		ATOM	3553		TRP A		19.554	24.896	77.165	1.00 26.16
		AT ON	2223	NET	TRP A	44/	20.654	23.217	78.197	1.00 27.23

5		MOTA	3554	CE2	TRP A	447	20.822	24.476	77.660	1.00 29.00
		MOTA	3555		TRP A		19.435	26.162	76.607	1.00 27.56
		MOTA	3556		TRP A		21.954	25.290	77.583	1.00 27.95
	•	ATOM	3557		TRP A		20.554	26.966	76.538	1.00 29.93
	5	ATOM	3558		TRP A		21.792	26.539	77.035	1.00 30.16
		ATOM	3559	N	LEU A		14.029	24.034	76.893	1.00 26.54
10		MOTA	3560	CA	LEU A		12.896	24.421	76.052	1.00 26.92
10		ATOM	3561	С	LEU A		11.734	25.064	76.779	1.00 36.15
	10	MOTA	3562	0	LEU A		11.089	26.031	76.304	1.00 31.19
	10	ATOM	3563	CB	LEU A		12.338	23.197	75.307	1.00 25.26
		ATOM	3564	CG.	LEU A		13.311	22.545	74.332	1.00 28.29
		ATOM	3565		LEU A		12.597	21.455	73.530	1.00 30.49
		ATOM	3566		LEU A		13.879	23.576	73.375	1.00 21.94
15	15	ATOM	3567	N	TYR A		11.472	24.455	77.924	1.00 33.14
•	15	ATOM	3568	CA	TYR A		10.373	24.835	78.747	1.00 30.64
		ATOM	3569	C	TYR A		10.646	25.525	80.041	1.00 34.31
		ATOM	3570	0	TYR A		9.750	26.191	80.529	1.00 41.98
		MOTA	3571	CB	TYR A		9.400	23.674	78.916	1.00 29.14
	20	ATOM	3572	CG	TYR A		9.212	23.089	77.556	1.00 26.50
	20	ATOM	3573		TYR A		8.762	23.869	76.485	1.00 24.36
20		ATOM	3574		TYR A		9.560	21.762	77.325	1.00 28.48
		ATOM	3575 3576		TYR A		8.626	23.331	75.202	1.00 17.56
		ATOM ATOM	3577	CE2	TYR A		9.427	21.205	76.054	1.00 29.93
	25	ATOM	3578	OH	TYR A		8.959	21.988	74.998	1.00 33.65
	25	ATOM	3579	N	SER A		8.840	21.415	73.762	1.00 39.47
		ATOM	3580	CA	SER A		11.806	25.413	80.644	1.00 22.72
05		ATOM	3581	C	SER A		11.902 12.278	26.149	81.900	1.00 21.21
25		ATOM	3582	o	SER A		12.966	27.625 28.035	81.749	1.00 23.98
	30	ATOM	3583	СВ	SER A		12.666	25.436	80.810	1.00 27.17
	30	ATOM	3584	OG	SER A		12.540	24.046	83.010	1.00 24.83 1.00 36.29
		ATOM	3585	N	PRO A		11.806	28.430	82.871 82.689	
		ATOM	3586	CA	PRO A		12.111	29.840	82.669	1.00 19.76
		ATOM	3587	c	PRO A		13.461	29.988	83.271	1.00 18.20 1.00 21.72
30	35	ATOM	3588	ŏ	PRO A		14.022	29.015	83.742	1.00 21.72
	55	ATOM	3589	СВ	PRO A		11.185	30.485	83.695	
		ATOM	3590	CG	PRO A		10.836	29.390	84.677	1.00 18.85 1.00 23.13
		ATOM	3591	CD	PRO A		11.002	28.078	83.900	1.00 23.13
		ATOM	3592	N	GLY A		13.959	31.212	83.307	1.00 13.01
	40	ATOM	3593	CA	GLY A		15.241	31.444	83.922	1.00 19.09
		ATOM	3594	C	GLY A		16.382	31.107	83.016	1.00 26.20
35		ATOM	3595	ō	GLY A		16.191	30.916	81.819	1.00 27.37
		ATOM	3596	N	LEU A		17.557	31.057	83.650	1.00 25.48
		ATOM	3597	CA	LEU A		18.843	30.750	83.029	1.00 25.32
	45	ATOM	3598	С	LEU A		18.906	29.322	82.629	1.00 26.21
		ATOM	3599	0	LEU A		18.400	28.458	83.322	1.00 25.04
		ATOM	3600	СВ	LEU A		20.042	31.119	83.938	1.00 25.46
40		ATOM	3601	ÇG	LEU A		20.280	32.632	83.904	1.00 31.82
40		ATOM	3602	CD1	LEU A	453	21.019	33.087	85.119	1.00 31.78
	50	ATOM	3603	CD2	LEU A	453	21.046	33.056	82.651	1.00 41.50
		ATOM	3604	N	PRO A	454	19.510	29.082	81.489	1.00 22.97
		ATOM	3605	CA	PRO A	454	19.585	27.747	81.003	1.00 21.60
		ATOM	3606	С	PRO A	454	20.145	26.890	82.075	1.00 26.94
		ATOM	3607	0	PRO A	454	20.923	27.359	82.893	1.00 29.09
45	55	ATOM	3608	CB	PRO A	454	20.489	27.780	79.768	1.00 22.34
		ATOM	3609	CG	PRO A		20.777	29.232	79.470	1.00 23.69
		ATOM	3610	CD	PRO A	454	20.136	30.054	80.556	1.00 20.82
		ATOM	3611	N	PRO A	455	19.721	25.648	82.067	1.00 25.61
	44	ATOM	3612	CA	PRO A	455	20.167	24.683	83.031	1.00 24.27
	60	ATOM	3613	С	PRO A	455	21.661	24.568	82.991	1.00 30.95
		ATOM	3614	0	PRO A	455	22.225	24.062	83.920	1.00 33.47
50		ATOM	3615	CB	PRO A	455	19.631	23.320	82.592	1.00 25.04
		ATOM	3616	CG	PRO A		19.149	23.497	81.162	1.00 33.02
		ATOM	3617	CD	PRO A	455	19.111	25.005	80.888	1.00 28.49

5		MOTA	3618	N.	ILE A	456	22.305	25.002	81.911	1.00 27.91
		ATOM	3619	CA	ILE A		23.764	24.893	81.821	1.00 27.82
		ATOM	3620	Ċ.	ILE A		24.395	26.057	81.077	1.00 27.02
		ATOM	3621	ō	ILE A		23.737	26.769	80.293	1.00 37.01
	5	ATOM	3622	CB	ILE A		24.228	23.540	81.259	1.00 37.01
	-	ATOM	3623		ILE A		25.721	23.305	81.417	1.00 29.78
		ATOM	3624		ILE A		23.865	23.369	79.788	1.00 32.96
10		MOTA	3625		ILE A		26.054	21.852	81.116	1.00 32.30
		ATOM	3626	N	LYS A		25.680	26.252	81.334	1.00 23.34
	10	ATOM	3627	CA	LYS A		26.405	27.335	80.707	1.00 30.32
		ATOM	3628	c	LYS A		27.515	26.808	79.835	1.00 30.21
		ATOM	3629	Ō	LYS A		28.328	26.037	80.273	1.00 33.07
		ATOM	3630	ČВ	LYS A		26.953	28.264	81.749	1.00 32.38
		ATOM	3631	CG	LYS A		27.818	29.327	81.121	1.00 34.64
15	15	ATOM	3632	CD	LYS A		28.288	30.306	82.166	1.00 13.41
		ATOM	3633	CE	LYS A		28.803	31.596	81.565	1.00 18.04
		ATOM	3634	NZ	LYS A		28.974	32.643	82.595	1.00 26.77
		ATOM	3635	N	PRO A		27.567	27.208	78.589	1.00 27.50
•		ATOM	3636	CA	PRO A		28.630	26.675	77.737	1.00 26.85
	20	ATOM	3637	c c	PRO A		29.994	27.147	78.185	1.00 26.89
00		ATOM	3638	ŏ	PRO A		30.128	27.876	79.167	
20		ATOM	3639	СВ	PRO A		28.335	27.191	76.316	1.00 24.86
		ATOM	3640	CG	PRO A		26.952	27.191		1.00 29.41
		ATOM	3641	CD	PRO A		26.574	28.044	76.375	1.00 33.24
	25	ATOM	3642	N	ASN A				77.848	1.00 26.12
	23	ATOM	3643	CA			31.005	26.754	77.440	1.00 22.13
		ATOM	3644		ASN A		32.359	27.191	77.735	1.00 22.29
25				C	ASN A		32.751	28.325	76.820	1.00 30.27
25		ATOM	3645	0	ASN A		32.451	28.296	75.617	1.00 32.89
	30	ATOM ATOM	3646 3647	CB	ASN A		33.315	26.060	77.494	1.00 25.03
	50			CG	ASN A		32.766	24.846	78.155	1.00 49.54
		MOTA	3648		ASN A		32.618	24.822	79.383	1.00 50.09
		MOTA	3649		ASN A		32.411	23.870	77.332	1.00 38.39
		MOTA	3650	N	TYR A		33.448	29.316	77.380	1.00 25.58
30	35	MOTA	3651	CA	TYR A		33.851	30.493	76.625	1.00 23.89
30	33	MOTA	3652	С	TYR A		35.298	30.853	76.745	1.00 34.20
		ATOM	3653	0	TYR A		35.849	30.862	77.839	1.00 35.27
		MOTA	3654	СB	TYR A		33.120	31.708	77.171	1.00 24.38
		ATOM	3655	CG	TYR A		31.636	31.631	77.024	1.00 26.98
	40	MOTA	3656		TYR A		31.029	32.011	75.829	1.00 30.69
	40	ATOM	3657	CD2	TYR A		30.838	31.168	78.064	1.00 25.70
35		ATOM	3658	CE1			29.644	31.952	75.684	1.00 28.77
		ATOM	3659	CE2	TYR A		29.453	31.096	77.938	1.00 25.24
		MOTA	3660	CZ	TYR A		28.863	31.496	76.741	1.00 24.49
	45	ATOM	3661	OH	TYR A		27.519	31.443	76.587	1.00 28.39
	43	ATOM	3662	N	ASP A		35.893	31.227	75.616	1.00 30.58
		MOTA	3663	CA	ASP A		37.268	31.640	75.654	1.00 27.51
		ATOM	3664	С	ASP A		37.319	32.941	76.464	1.00 23.53
40		ATOM	3665	0	ASP A		36.377	33.704	76.396	1.00 26.62
	50	MOTA	3666	CB	ASP A		37.821	31.784	74.218	1.00 27.30
	50	ATOM	3667	CG	ASP A		39.137	32.466	74.260	1.00 32.53
		MOTA	3668		ASP A		39.262	33.672	74.334	1.00 39.66
		ATOM	3669		ASP A		40.130	31.628	74.306	1.00 44.34
		ATOM	3670	N	MET A		38.375	33.234	77.224	1.00 17.26
		ATOM	3671	CA	MET A		38.396	34.511	78.008	1.00 18.66
45	55	ATOM	3672	С	MET A		39.299	35.634	77.485	1.00 24.02
		ATOM	3673	0	MET A	462	39.336	36.738	78.011	1.00 24.56
		ATOM	3674	CB	MET A	462	38.818	34.186	79.431	1.00 22.99
		ATOM	3675	CG	MET A		37.808	33.209	80.025	1.00 28.98
	<i>c</i> 0	ATOM	3676	SD	MET A	462	36.166	33.969	79.951	1.00 33.22
	60	ATOM	3677	CE	MET A		36.420	35.300	01.153	1.00 27.89
		ATOM	3678	N	THR A		40.067	35.348	76.461	1.00 22.57
50		ATOM	3679	CA	THR A	463	41.015	36.285	75.911	1.00 22.64
		ATOM	3680	С	THR A	463	40.690	37.738	75.961	1.00 33.12
		ATOM	3681	0	THR A	463	41.372	38.493	76.640	1.00 35.27

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5		ATOM	3682	CB.	THR A 46	53 41.574	35.929	74.536	1.00 29.80
		ATOM	3683		THR A 46			74.509	1.00 26.74
		ATOM	3684		THR A 46			74.224	1.00 18.79
		MOTA	3685	N	LEU A 46	39.700		75.177	1.00 30.50
	5	ATOM	3686	CA	LEU A 46			75.061	1.00 29.15
	•	ATOM	3687	С	LEU A 46			76.216	1.00 34.24
		ATOM	3688	ō	LEU A 46			76.422	1.00 37.12
10		ATOM	3689	СВ	LEU A 46			73.743	1.00 29.20
		ATOM	3690	CG	LEU A 46			72.527	1.00 23.20
	10	ATOM	3691		LEU A 46			71.217	1.00 33.73
	10	ATOM	3692		LEU A 46			72.499	1.00 26.22
		ATOM	3693	N	THR A 46			76.964	1.00 20.22
		MOTA	3694	CA	THR A 46				
		ATOM	3695	C	THR A 46			76.103 79.324	1.00 28.58
15	15	ATOM	3696	ŏ	THR A 46			80.030	1.00 30.69 1.00 31.27
	13	ATOM	3697	CB	THR A 46			78.372	
			3698						1.00 35.85
		MOTA			THR A 46			77.296	1.00 50.93
		MOTA	3699		THR A 46			79.690	1.00 26.34
	20	MOTA	3700	N	ASN A 46			79.568	1.00 24.40
0.	20	ATOM	3701	CA	ASN A 46			80.688	1.00 23.11
20		MOTA	3702	С	ASN A 46			80.967	1.00 28.37
		MOTA	3703	0	ASN A 46			82.120	1.00 27.03
		MOTA	3704	CB	ASN A 46			80.629	1.00 20.30
		ATOM	3705	CG	ASN A 46			81,155	1.00 32.26
	25	MOTA	3706		ASN A 46			80.723	1.00 29.29
		ATOM	3707	ND2	ASN A 46	56 39 . 775	37.015	82.111	1.00 28.19
		MOTA	3708	N	ALA A 46	57 40.306	41.666	79.967	1.00 27.97
25		MOTA	3709	CA	ALA A 46	67 40.587	43.079	80.295	1.00 26.66
		MOTA	3710	С	ALA A 46	57 39.352	43.827	80.720	1.00 31.78
	30	MOTA	3711	0	ALA A 46	57 39.406	44.845	81.393	1.00 31.71
		ATOM	3712	CB	ALA A 46	57 41.369	43.837	79.256	1.00 25.99
		ATOM	3713	N	CYS A 46	58 38.217	43.277	80.336	1.00 28.06
		ATOM	3714	CA	CYS A 46	58 36.942	43.862	80.693	1.00 25.80
		ATOM	3715	С	CYS A 46	58 36.668		82.165	1.00 26.47
30	35	ATOM	3716	0	CYS A 46			82.963	1.00 27.99
		ATOM	3717	CB	CYS A 46			79.696	1.00 24.56
		MOTA	3718	SG	CYS A 46			78.049	1.00 27.76
		ATOM	3719	N	ILE A 46			82.540	1.00 24.34
		ATOM	3720	CA	ILE A 46			83.921	1.00 25.23
	40	ATOM	3721	С	ILE A 46			84.876	1.00 28.13
		ATOM	3722	0	ILE A 46			85.950	1.00 29.54
35		ATOM	3723	CB	ILE A 46			84.068	1.00 27.23
		ATOM	3724		ILE A 46			83.112	1.00 26.94
		ATOM	3725		ILE A 46			85.496	1.00 25.56
	45	ATOM	3726		ILE A 40			83.085	1.00 45.50
	•••	ATOM	3727	N	ALA A 4			84.534	1.00 23.28
		ATOM	3728	CA	ALA A 4			85.461	1.00 23.23
40		ATOM	3729	c.	ALA A 4			85.808	1.00 30.29
40		ATOM	3730	Ö	ALA A 4			86.986	1.00 30.29
	50	ATOM	3731	СВ	ALA A 4				
	50	ATOM	3732		LEU A 4			85.074 84.759	1.00 21.98
		ATOM	3733	N	LEU A 4				1.00 23.53
				CA				84.834	1.00 18.39
		ATOM	3734	C	LEU A 4			85.569	1.00 26.57
15	55	ATOM	3735	0	LEU A 4			86.462	1.00 30.48
45	33	ATOM	3736	CB	LEU A 4			83.444	1.00 15.51
		MOTA	3737	CG	LEU A 4			83.539	1.00 24.20
		MOTA	3738		LEU A 4			84.513	1.00 24.86
		ATOM	3739		LEU A 4			82.156	1.00 26.35
	~	MOTA	3740	N	SER A 4			85.222	1.00 25.31
	60	MOTA	3741	CA	SER A 4			85.901	1.00 27.56
50		ATOM	3742	С	SER A 4	72 35.26	46.477	87.396	1.00 33.46
50		MOTA	3743	0	SER A 4	72 34.80	47.292	88.214	1.00 32.85
		ATOM	3744	СВ	SER A 4	72 33.989	45.714	85.393	1.00 32.06
		ATOM	3745	OG	SER A 4	72 34.49	44.774	84.470	1.00 48.56

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5		ATOM	3746	Ν.	GLN A	473	35.911	45.350	87.736	1.00 27.52
		ATOM '	3747	CA	GLN A	473	36.170	44.971	89.108	1.00 24.10
		ATOM	3748	С	GLN A	473	36.866	46.096	89.836	1.00 25.18
		ATOM	3749	0	GLN A	473	36.534	46.458	90.969	1.00 21.62
	5	ATOM	3750	СВ	GLN A	473	36.994	43.671	89.148	1.00 25.86
		ATOM	3751	CG	GLN A	473	36.128	42.402	89.118	1.00 32.72
10		MOTA	3752	CD	GLN A	473	34.970	42.504	90.090	1.00 46.08
10		MOTA	3753	OE1	GLN A	473	35.165	42.422	91.308	1.00 40.73
		ATOM	3754	NE2	GLN A	473	33.761	42.692	89.559	1.00 28.28
	10	ATOM	3755	N	ARG A	474	37.855	46.656	89.161	1.00 24.00
		ATOM	3756	CA	ARG A	474	38.562	47.765	89.779	1.00 24.46
		ATOM	3757	С	ARG A	474	37.609	48.893	90.141	1.00 29.31
		ATOM	3758	0	ARG A	474	37.620	49.447	91.242	1.00 33.13
15		ATOM	3759	CB	ARG A	474	39.682	48.290	88.898	1.00 20.19
,,,	15	MOTA	3760	CG	ARG A	474	40.866	47.352	88.831	1.00 28.48
		ATOM	3761	CD	ARG A	474	41.871	47.869	87.832	1.00 34.41
		ATOM	3762	NE	ARG A	474	42.258	49.245	88.093	1.00 40.09
		MOTA	3763	CZ	ARG A	474	42.927	49.938	87.185	1.00 51.25
		ATOM	3764	NHl	ARG A	474	43.220	49.376	86.019	1.00 24.79
	20	MOTA	3765	NH2	ARG A	474	43.316	51.199	87.444	1.00 20.43
20		ATOM	3766	N	TRP A	475	36.791	49.259	89.178	1.00 25.32
		ATOM	3767	CA	TRP A	475	35.862	50.332	89.400	1.00 26.77
		ATOM	3768	С	TRP A	475	34.881	49.962	90.474	1.00 27.52
		ATOM	3769	0	TRP A	475	34.749	50.633	91.475	1.00 29.64
	25	ATOM	3770	CB	TRP A	475	35.199	50.804	88.093	1.00 27.95
		MOTA	3771	CG	TRP A	475	36.047	51.819	87.361	1.00 32.11
		ATOM	3772	CD1	TRP A	475	36.873	51.592	86.298	1.00 35.65
25		ATOM	3773	CD2	TRP A	475	36.161	53.217	87.648	1.00 31.62
		MOTA	3774	NE1	TRP A	475	37.484	52.748	85.904	1.00 34.92
	30	ATOM	3775	CE2	TRP A	475	37.054	53.763	86.707	1.00 36.16
		MOTA	3776	CE3	TRP A	475	35.588	54.040	88.606	1.00 32.63
		ATOM	3777	CZ2	TRP A	475	37.372	55.112	86.719	1.00 36.24
		MOTA	3778	CZ3	TRP A	475	35.897	55.375	88.616	1.00 34.74
		ATOM	3779	CH2	TRP A	475	36.777	55.901	87.685	1.00 35.77
30	35	ATOM	3780	N	ILE A	476	34.234	48.847	90.279	1.00 26.36
		ATOM	3781	CA	ILE A	476	33.268	48.386	91.235	1.00 28.33
		ATOM	3782	С	ILE A	476	33. 7 71	48.315	92.681	1.00 34.20
		ATOM	3783	0	ILE A	476	33.056	48.595	93.637	1.00 36.89
		ATOM	3784	CB	ILE A	476	32.722	47.070	90.761	1.00 32.23
	40	ATOM	3785	CG1	ILE A	476	31.993	47.308	89.443	1.00 30.49
35		ATOM	3786	CG2	ILE A	476	31.864	46.376	91.851	1.00 34.86
33		ATOM	3787	CD1	ILE A	476	31.595	46.005	88.756	1.00 33.04
		ATOM	3788	N	THR A	477	35.010	47.934	92.860	1.00 27.27
		ATOM	3789	CA	THR A	477	35.558	47.846	94.194	1.00 24.15
	45	ATOM	3790	С	THR A	477	36.416	49.052	94.523	1.00 27.30
		ATOM	3791	0	THR A	477	37.120	49.065	95.519	1.00 27.36
		ATOM	3792	CB	THR A		36.402	46.578	94.257	1.00 32.13
40		ATOM	3793	OG1	THR A	477	37.593	46.848	93.557	1.00 29.48
		ATOM	3794	CG2	THR A	477	35.634	45.470	93.530	1.00 16.94
	50	ATOM	3795	N	ALA A	478	36.371	50.097	93.695	1.00 22.33
		ATOM	3796	CA	ALA A	478	37.164	51.260	93.988	1.00 20.44
		ATOM	3797	С	ALA A	478	36.890	51.843	95.390	1.00 32.94
		MOTA	3798	0	АЬА А	478	35.786	51.756	95.922	1.00 34.38
		ATOM	3799	CB	ALA A	478	36.938	52.343	92.942	1.00 19.26
45	55	ATOM	3800	N	LYS A	479	37.931	52.469	95.970	1.00 29.65
		MOTA	3801	CA	LYS A	479	37.899	53.168	97.243	1.00 27.30
		ATOM	3802	С	LYS A	479	38.575	54.512	97.051	1.00 36.54
		MOTA	3803	0	LYS A	479	39.378	54.692	96.118	1.00 34.13
		ATOM	3804	CB	LYS A	479	38.457	52.410	98.417	1.00 28.01
	60	MOTA	3805	CG	LYS A	479	37.696	51.116	98.631	1.00 51.38
		ATOM	3806	CD	LYS A		37.115		100.021	1.00 67.24
50		MOTA	3807	CE	LYS A	479	35.804	50.103	99.931	1.00 87.12
		MOTA	3808	NZ	LYS A		35.711		100.841	1.00 85.55
		ATOM	3809	N	GLU A		38.241	55.477	97.900	1.00 36.30
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5		ATOM	3810	CA	GLU A 4	180	38.843	56.793	97.751	1.00 34.79
		ATOM	3811	С	GLU A 4	180	40.261	56.707	97.220	1.00 34.79
		ATOM	3812	0	GLU A 4	180	40.613	57.332	96.234	1.00 34.10
		ATOM	3813	CB	GLU A 4	180	38.899	57.565	99.078	1.00 36.21
	5	ATOM	3814	CG	GLU A 4	180	37.709	58.500	99.303	1.00 63.85
		ATOM	3815	CD	GLU A 4	180	37.601	59.511	98.214	1.00100.00
		ATOM	3816	OE1	GLU A 4	180	38.457	59.648	97.357	1.00100.00
10		ATOM	3817	OE2	GLU A 4	180	36.491	60.209	98.288	1.00100.00
		ATOM	3818	N	ASP A 4	181	41.080	55.946	97.904	1.00 24.69
	10	ATOM	3819	CA	ASP A 4		42.451	55.860	97.519	1.00 23.87
		ATOM	3820	С	ASP A 4	181	42.771	55.314	96.132	1.00 34.51
		ATOM	3821	0	ASP A 4	181	43.925	55.312	95.721	1.00 39.44
		ATOM	3822	СВ	ASP A 4	181	43.262	55.155	98.611	1.00 25.29
45		ATOM	3823	CG	ASP A 4	181	43.072	53.668	98.575	1.00 39.58
15	15	ATOM	3824	OD1	ASP A 4	181	42.471	53.029	97.708	1.00 46.00
		MOTA	3825	OD2	ASP A 4	181	43.698	53.107	99.567	1.00 39.59
		ATOM	3826	N	ASP A 4		41.788	54.881	95.373	1.00 30.70
		ATOM	3827	CA	ASP A 4		42.098	54.379	94.024	1.00 31.73
		ATOM	3828	С	ASP A 4		41.725	55.307	92.859	1.00 34.17
	20	ATOM	3829	0	ASP A 4	182	42.158	55.150	91.717	1.00 35.45
20		ATOM	3830	СВ	ASP A 4	182	41.399	53.022	93.756	1.00 33.31
20		ATOM	3831	CG	ASP A 4		41.686	51.970	94.779	1.00 38.90
		ATOM	3832		ASP A 4		42.810	51.514	94.992	1.00 42.45
		ATOM	3833		ASP A 4		40.606	51.625	95.440	1.00 40.17
	25	ATOM	3834	N	LEU A 4		40.863	56.246	93.146	1.00 29.93
		MOTA	3835	CA	LEU A 4		40.352	57.159	92.160	1.00 27.80
		ATOM	3836	С	LEU A 4		41.434	57.943	91.410	1.00 40.70
25		ATOM	3837	0	LEU A 4		41.386	58.102	90.180	1.00 40.76
20		ATOM	3838	СВ	LEU A 4		39.265	58.049	92.819	1.00 22.54
	30	ATOM	3839	CG	LEU A 4		38.148	57.240	93.488	1.00 20.75
		ATOM	3840		LEU A 4		37.170	58.165	94.197	1.00 19.29
		ATOM	3841		LEU A 4		37.389	56.467	92.414	1.00 21.46
		ATOM	3842	N	ASN A		42.410	58.446	92.162	1.00 36.15
		ATOM	3843	CA	ASN A		43.459	59.225	91.571	1.00 34.08
30	35	ATOM	3844	C	ASN A		44.168	58.524	90.429	1.00 39.51
		ATOM	3845	ō	ASN A		44.456	59.091	89.359	1.00 38.59
		MOTA	3846	СВ	ASN A		44.495	59.602	92.618	1.00 34.26
		ATOM	3847	CG	ASN A		45.807	59.955	91.941	1.00100.00
		ATOM	3848		ASN A		45.878	60.940	91.171	1.00100.00
	40	ATOM	3849		ASN A		46.836	59.134	92.186	1.00100.00
		ATOM	3850	N	SER A 4		44.472	57.268	90.698	1.00 35.37
35		ATOM	3851	CA	SER A		45.202	56.417	89.791	1.00 32.79
		ATOM	3852	C	SER A		44.522	56.140	88.484	1.00 32.26
		ATOM	3853	ō	SER A		45.159	55.925	87.463	1.00 32.44
	45	ATOM	3854	CB	SER A		45.565	55.132	90.477	1.00 38.65
		MOTA	3855	OG	SER A		46.040	55.437	91.777	1.00 62.66
		MOTA	3856	N	PHE A		43.222	56.110	88.491	1.00 27.13
40		ATOM	3857	CA	PHE A		42.631	55.809	87.233	1.00 28.26
40		ATOM	3858	С	PHE A		43.193	56.772	86.264	1.00 32.12
	50	ATOM	3859	0	PHE A		43.423	57.910	86.604	1.00 32.02
		ATOM	3860	СВ	PHE A		41.101	55.819	87.198	1.00 31.01
		ATOM	3861	CG	PHE A		40.471	54.807	88.132	1.00 27.04
		ATOM	3862		PHE A		40.504	53.425	87.911	1.00 22.43
		ATOM	3863	CD2	PHE A	186	39.805	55.293	89.253	1.00 21.40
45	55	ATOM	3864		PHE A		39.896	52.538	88.804	1.00 19.69
70		ATOM	3865		PHE A		39.224	54.426	90.174	1.00 19.20
		ATOM	3866	CZ	PHE A		39.245	53.051	89.927	1.00 15.13
		ATOM	3867	N	ASN A		43.455	56.279	85.089	1.00 34.97
		ATOM	3868	CA	ASN A		44.032	57.092	84.070	1.00 34.97
	60	ATOM	3869	c.	ASN A		43.491	56.622	82.758	1.00 43.55
		ATOM	3870	ō	ASN A		42.951	55.537	82.604	1.00 46.30
50		ATOM	3871	СВ	ASN A		45.591	57.038	84.085	1.00 43.93
		ATOM	3872	CG	ASN A		46.196	58.169	83.302	1.00 56.10
		ATOM	3873		ASN A		46.057	58.189	82.077	1.00 30.10
		OI'I	5575	ODI	AND A	,	.0.00,	50.103	32.017	4.00 4Z.1Z

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5		ATOM	3874	•	ASN A		46.829	59.112	84.007	1.00 65.62
		ATOM	3875 3876	N CA	ALA A		43.662	57.435	81.781	1.00 39.34
		ATOM ATOM	3877	CA	ALA A		43.201 44.024	57.055	80.472	1.00 38.25
	5	ATOM	3878	Ö	ALA A		43.596	55.900 55.317	79.809 78.834	1.00 43.58
	,	ATOM	3879	СВ	ALA A		43.153	58.314	79.621	1.00 44.11 1.00 37.54
		ATOM	3880	N	THR A		45.207	55.555	80.314	1.00 37.34
10		ATOM	3881	CA	THR A		45.996	54.499	79.715	1.00 36.16
		ATOM	3882	c	THR A		45.270	53.181	79.792	1.00 45.74
	10	ATOM	3883	0	THR A		45.476	52.233	79.057	1.00 47.78
		ATOM	3884	CB	THR A		47.296	54.458	80.503	1.00 31.01
		ATOM	3885	0G1	THR A	489	46.961	54.457	81.872	1.00 35.33
		ATOM	3886	CG2	THR A	489	47.993	55.771	80.229	1.00 28.28
15		ATOM	3887	N	ASP A	490	44.337	53.182	80.708	1.00 46.75
15	15	ATOM	3888	CA	ASP A	490	43.560	52.018	80.972	1.00 51.49
		MOTA	3889	С	ASP A		42.759	51.515	79.786	1.00 52.21
		ATOM	3890	0	ASP A		42.396	50.342	79.651	1.00 54.75
		ATOM	3891	CB	ASP A		42.676	52.345	82.184	1.00 54.04
	20	MOTA	3892	CG	ASP A		43.413	52.884	83.380	1.00 53.83
	20	MOTA	3893		ASP A		44.621	52.777	83.616	1.00 62.93
20		MOTA	3894		ASP A		42.565	53.446	84.165	1.00 35.66
		ATOM	3895	N	LEU A		42.486	52.450	78.938	1.00 42.42
		ATOM	3896	CA	LEU A		41.752	52.250	77.723	1.00 43.54
	25	ATOM	3897	C	LEU A		42.712	51.977	76.585	1.00 43.97
	23	ATOM	3898	0	LEU A		42.340	51.438	75.588	1.00 42.53
		ATOM	3899	CB	LEU A		40.984	53.528	77.421	1.00 44.89
45		ATOM ATOM	3900	CG	LEU A		39.794	53.747	78.338	1.00 48.31
25		ATOM	3901 3902		LEU A		38.558	54.171	77.552	1.00 49.16
	30	ATOM	3903	N	LEU A LYS A		39.377 43.958	52.494 52.403	79.125 76.754	1.00 39.24
	50	MOTA	3904	CA	LYS A		44.999	52.320	75.696	1.00 42.32 1.00 44.57
		ATOM	3905	c	LYS A		44.826	51.165	74.680	1.00 49.08
		ATOM	3906	ŏ	LYS A		44.810	51.343	73.473	1.00 49.66
		ATOM	3907	CB	LYS A		46.359	52.177	76.401	1.00 48.47
30	35	MOTA	3908	CG	LYS A		47.487	52.883	75.629	1.00 88.73
		ATOM	3909	CD	LYS A		48.852	52.537	76.197	1.00100.00
		MOTA	3910	CE	LYS A		48.786	51.460	77.300	1.00100.00
		ATOM	3911	NZ	LYS A		50.103	50.896	77.541	1.00100.00
		MOTA	3912	N	ASP A		44.711	49.917	75.227	1.00 41.86
	40	MOTA	3913	CA	ASP A	493	44.664	48.740	74.372	1.00 40.17
05		MOTA	3914	С	ASP A	493	43.220	48.162	74.215	1.00 44.29
35		MOTA	3915	0	ASP A		43.031	46.973	73.889	1.00 42.00
		MOTA	3916	CB	ASP A		45.560	47.699	75.015	1.00 41.52
	45	MOTA	3917	CG	ASP A		47.021	48.130	74.956	1.00 67.01
	45	ATOM	3918		ASP A		47.467	48.451	73.856	1.00 77.10
		ATOM	3919		ASP A		47.678	48.131	75.984	1.00 57.19
		ATOM	3920	N	LEU A		42.193	49.005	74.475	1.00 40.69
40		ATOM	3921	CA	LEU A		40.789	48.512	74.526	1.00 36.32
	50	ATOM	3922	c	LEU A		39.992	48.877	73.245	1.00 37.76
	50	ATOM	3923	0	LEU A		39.897	50.029	72.863	1.00 38.93
		ATOM	3924 3925	CB	LEU A		40.098	49.125	75.733	1.00 32.52
		ATOM ATOM	3926	CG	LEU A		40.376	48.433	77.063	1.00 30.66
		ATOM	3927		LEU A		39.229 40.611	48.580	78.052	1.00 30.39
45	55	ATOM	3928	N N	SER A		39.477	46.925 47.825	76.918 72.631	1.00 23.54
45		ATOM	3929	CA	SER A		38.674	47.623	72.631	1.00 25.56 1.00 22.23
		ATOM	3930	C	SER A		37.344	48.670	71.856	1.00 22.23
		ATOM	3931	Ö	SER A		36.968	48.706	73.038	1.00 31.27
		ATOM	3932	СВ	SER A		38.380	46.705	70.795	1.00 31.21
	60	ATOM	3933	OG	SER A		37.192	46.143	71.317	1.00 20.66
		ATOM	3934	N	SER A		36.627	49.184	70.865	1.00 29.48
50		ATOM	3935	CA	SER A		35.363	49.821	71.139	1.00 26.67
		ATOM	3936	c	SER A		34.495	48.747	71.744	1.00 29.54
		ATOM	3937	ŏ	SER A		33.744	48.960	72.697	1.00 24.80
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5		ATOM	3938	CB ·	SER A 496	34.760	50.441	69.894	1.00 24.67
		ATOM	3939	OG	SER A 496	33.749	49.597	69.397	1.00 48.80
		MOTA	3940	N	HIS A 497		47.547	71.219	1.00 26.61
	_	ATOM	3941	CA	HIS A 497		46.383	71.750	1.00 29.22
	5	ATOM	3942	С	HIS A 497		46.148	73.275	1.00 37.24
		ATOM	3943	0	HIS A 49		45.863	74.041	1.00 38.21
10		ATOM	3944	CB	HIS A 49		45.106	70.978	1.00 30.69
		ATOM	3945	CG	HIS A 497		45.348	69.545	1.00 34.29
	10	ATOM	3946		HIS A 49		45.204	68.962	1.00 35.42
	10	ATOM	3947		HIS A 49		45.833	68.622	1.00 36.68
		ATOM	3948		HIS A 49		45.531	67.702	1.00 35.05
		ATOM	3949		HIS A 49'		45.932	67.462	1.00 35.88
		ATOM ATOM	3950 3951	N CA	GLN A 498		46.243 46.008	73.715 75.094	1.00 33.56 1.00 29.69
15	15	ATOM	3952	C	GLN A 49		47.122	75.965	1.00 27.11
	13	ATOM	3953	ò	GLN A 49		46.930	77.089	1.00 23.92
		ATOM.	3954	СВ	GLN A 49		45.659	75.248	1.00 29.95
		ATOM	3955	CG	GLN A 49		44.317	74.544	1.00 25.78
		ATOM	3956	CD	GLN A 49		44.084	74.535	1.00 28.64
•	20	ATOM	3957		GLN A 49		44.891	73.960	1.00 26.62
20		ATOM	3958		GLN A 49		43.049	75.218	1.00 20.96
		ATOM	3959	N	LEU A 49		48.301	75.431	1.00 27.13
		ATOM	3960	CA	LEU A 49		49.396	76.229	1.00 29.32
		ATOM	3961	C	LEU A 49		49.162	76.632	1.00 28.39
	25	ATOM	3962	0	LEU A 49		49.361	77.780	1.00 29.41
		MOTA	3963	CB	LEU A 49		50.709	75.436	1.00 31.70
		MOTA	3964	CG	LEU A 49	36.242	51.512	75. 7 88	1.00 39.76
25		ATOM	3965	CD1	LEU A 49	9 37.335	50.572	76.278	1.00 42.91
		MOTA	3966	CD2	LEU A 49	9 36.718	52.268	74.555	1.00 39.08
	30	ATOM	3967	N	ASN A 50	32.606	48.737	75.642	1.00 15.23
		ATOM	3968	CA	ASN A 50	31.213	48.508	75.828	1.00 13.44
		ATOM	3969	С	ASN A 50	30.919	47.455	76.864	1.00 18.98
		ATOM	3970	0	ASN A 50	0 29.997	47.602	77.705	1.00 19.01
30		ATOM	3971	CB	ASN A 50	0 30.604	48.129	74.476	1.00 12.21
30	35	ATOM	3972	CG	ASN A 50		48.214	74.426	1.00 37.49
		MOTA	3973		ASN A 50		49.151	74.930	1.00 36.17
		ATOM	3974		ASN A 50		47.218	73.787	1.00 18.34
		ATOM	3975	N	GLU A 50		46.366	76.743	1.00 14.20
	40	ATOM	3976	CA	GLU A 50		45.224	77.625	1.00 13.27
	40	MOTA	3977	С	GLU A 50		45.676	79.063	1.00 21.59
35		ATOM	3978	0	GLU A 50		45.463	80.009	1.00 25.02
		ATOM	3979	CB	GLU A 50		44.057	77.053	1.00 14.95
		ATOM	3980	CG	GLU A 50		42.827	77.989	1.00 30.40
	45	ATOM	3981	CD	GLU A 50		42.399	78.199	1.00 39.28
	7.7	ATOM ATOM	3982 3983		GLU A 50 GLU A 50		42.672 41.694	77.413 79.292	1.00 76.70 1.00 46.10
		ATOM	3984	N N	PHE A 50		46.400	79.232	1.00 48.10
40		ATOM	3985	CA	PHE A 50		46.952	80.530	1.00 18.07
70		ATOM	3986	c	PHE A 50		47.679	81.125	1.00 23.38
	50	ATOM	3987	ō	PHE A 50		47.491	82.301	1.00 21.47
	-	MOTA	3988	ČВ	PHE A 50		48.012	80.327	1.00 26.05
		ATOM	3989	ÇG	PHE A 50		49.082	81.393	1.00 30.41
		ATOM	3990		PHE A 50		48.781	82.662	1.00 29.68
		ATOM	3991		PHE A 50		50.402	81.132	1.00 39.16
45	55	ATOM	3992		PHE A 50		49.773	83.638	1.00 31.12
		ATOM	3993		PHE A 50		51.414	82.096	1.00 40.46
		ATOM	3994	CZ	PHE A 50		51.090	83.352	1.00 35.41
		MOTA	3995	N	LEU A 50		48.557	80.288	1.00 18.39
		ATOM	3996	CA	LEU A 50		49.343	80.692	1.00 22.78
	60	MOTA	3997	С	LEU A 50		48.491	81.178	1.00 31.04
50		MOTA	3998	0	LEU A 50		48.784	82.243	1.00 29.23
50		MOTA	3999	СВ	LEU A 50		50.325	79.619	1.00 24.68
		MOTA	4000	CG	LEU A 50		51.571	79.465	1.00 27.47
		ATOM	4001	CD1	LEU A 50	3 30.415	52.376	78.259	1.00 24.86

5		ATOM	4002	CD2	LEU A	503	30.860	52.420	80.733	1.00 20.54
		ATOM	4003	N	ALA A		29.012	47.444	80.378	1.00 27.79
		ATOM	4004	CA	ALA A		27.911	46.474	80.643	1.00 24.63
		ATOM	4005	c c	ALA A		28.140	45.752	81.939	1.00 27.71
	5	ATOM	4006	ō	ALA A		27.265	45.577	82.817	1.00 28.62
	•	ATOM	4007	СВ	ALA A		27.762	45.482	79.496	1.00 23.87
		MOTA	4008	N	GLN A		29.382	45.344	82.066	1.00 22.16
10		ATOM	4009	CA	GLN A		29.738	44.710	83.299	1.00 21.02
		ATOM	4010	c .	GLN A		29.489	45.737	84.423	1.00 31.26
	10	ATOM	4011	ō	GLN A		28.787	45.507	85.413	1.00 32.31
		ATOM	4012	СВ	GLN A		31.202	44.209	83.270	1.00 18.95
		ATOM	4013	CG	GLN A		31.367	42.881	82.495	1.00 13.72
		ATOM	4014	CD	GLN A		32.806	42.549	82.136	1.00 31.75
45		ATOM	4015		GLN A		33.796	42.969	82.768	1.00 43.14
15	15	ATOM	4016		GLN A		32.923	41.781	81.085	1.00 39.34
		ATOM	4017	N	THR A		30.056	46.918	84.263	1.00 25.95
		ATOM	4018	CA	THR A		29.855	47.864	85.302	1.00 23.64
		ATOM	4019	c	THR A		28.411	48.101	85.579	1.00 23.89
		ATOM	4020	ŏ	THR A		27.923	47.999	86.696	1.00 22.75
	20	ATOM	4021	СВ	THR A		30.600	49.130	85.008	1.00 23.72
20	20	ATOM	4022		THR A		31.938	48.749	84.742	1.00 27.18
20		ATOM	4023		THR A		30.502	49.961	86.260	1.00 27.18
		ATOM	4024	N	LEU A		27.727	48.408	84.518	1.00 17.92
		ATOM	4025	CA	LEU A		26.334	48.683	84.604	1.00 17.32
	25	ATOM	4026	C	LEU A		25.618	47.683	85.442	1.00 25.65
	LJ	ATOM	4027	Ö	LEU A		24.816	48.073	86.266	1.00 27.85
		ATOM	4028	СВ	LEU A		25.693	48.686	83.224	1.00 27.85
25		ATOM	4029	CG	LEU A		24.207	48.930	83.336	1.00 21.02
		ATOM	4030		LEU A		23.974	50.290	83.970	1.00 21.02
	30	ATOM	4031		LEU A		23.599	48.919	81.949	1.00 22.40
	30	ATOM	4032	N	GLN A		25.878	46.395	85.194	1.00 21.35
		ATOM	4033	CA	GLN A		25.215	45.333	85.979	1.00 18.08
		ATOM	4034	C	GLN A		25.386	45.561	87.508	1.00 34.24
		ATOM	4035	ō	GLN A		24.653	45.017	88.343	1.00 34.04
30	35	ATOM	4036	СВ	GLN A		25.713	43.917	85.608	1.00 10.94
	55	ATOM	4037	CG	GLN A		25.366	43.446	84.191	1.00 26.42
		ATOM	4038	CD.	GLN A		25.635	41.944	84.002	1.00 52.93
		ATOM	4039		GLN A		26.550	41.396	84.628	1.00 32.89
		ATOM	4040		GLN A		24.864	41.252	83.147	1.00 34.36
	40	ATOM	4041	N	ARG A		26.380	46.361	87.901	1.00 33.73
22	10	ATOM	4042	CA	ARG A		26.600	46.614	89.328	1.00 32.53
35		ATOM	4043	c .	ARG A		26.153	48.016	89.727	1.00 33.63
		ATOM	4044	ō	ARG A		26.509	48.522	90.777	1.00 31.08
		ATOM	4045	СВ	ARG A		28.055	46.440	89.760	1.00 29.22
	45	ATOM	4046	CG	ARG A		28.553	45.014	89.733	1.00 29.78
	1.5	ATOM	4047	CD	ARG A		27.744	44.054	90.609	1.00 30.86
		ATOM	4048	NE	ARG A		28.533	43.602	91.756	
40		ATOM	4049	CZ	ARG A		29.842	43.274	91.726	1.00 82.23
40		ATOM	4050		ARG A		30.579	43.315	90.613	1.00100.00
	50	ATOM	4051		ARG A		30.430	42.881	92.855	1.00 92.85
	50	ATOM	4052		ALA A			48.659	88.880	1.00 32.59
		ATOM	4053	CA	ALA A		24.952	49.985	89.215	1.00 32.53
		ATOM	4054	C	ALA A		24.151	49.845	90.479	1.00 34.97
		ATOM	4055	Ö	ALA A		23.601	48.785	90.693	1.00 37.57
45	55	ATOM	4056	СВ	ALA A		24.189	50.622		
	JJ	ATOM	4057	И	PRO A		24.174	50.856	88.063 91.334	1.00 32.91 1.00 25.14
		ATOM	4058	CA	PRO A		24.174	52.102	91.052	1.00 23.14
		ATOM	4059	CA	PRO A		26.217	52.102	91.694	
		ATOM	4059	0	PRO F					1.00 29.23
	60		4061	СВ	PRO P		26.445 24.102	51.601 53.169	92.723	1.00 28.16
	00	ATOM ATOM	4062		PRO A		23.316		91.818	1.00 21.55
50			4062	CG CD				52.432	92.886	1.00 28.68
		ATOM			PRO A		23.169	50.995	92.407	1.00 25.16
		ATOM	4064	N	LEU A		27.094	52.968	91.109	1.00 32.95
		ATOM	4065	CA	LEU A	1 312	28.394	53.188	91.686	1.00 33.42

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5		ATOM	4066	C .	LEU A	512	28.287	54.512	92.397	1.00 38.65
		ATOM	4067	0	LEU A		27.388	55.305	92.114	1.00 40.69
		ATOM	4068	CB	LEU A		29.453	53.350	90.587	1.00 34.40
		ATOM	4069	CG	LEU A		30.178	52.049	90.216	1.00 40.13
	5	ATOM	4070	CD1	LEU A	512	29.222	51.086	89.508	1.00 39.04
		ATOM	4071	CD2	LEU A	512	31.322	52.385	89.273	1.00 44.61
10		MOTA	4072	N	PRO A	513	29.196	54.781	93.312	1.00 31.05
10		ATOM	4073	CA	PRO A	513	29.167	56.058	94.008	1.00 27.16
		MOTA	4074	C	PRO A		29.296	57.203	93.019	1.00 23.76
	10	ATOM	4075	0	PRO A		30.121	57.182	92.118	1.00 27.17
		MOTA	4076	CB	PRO A		30.387	56.013	94.948	1.00 25.59
		ATOM	4077	CG	PRO A		30.702	54.542	95.149	1.00 27.14
		ATOM	4078	CD	PRO A		30.030	53.779	94.032	1.00 25.00
15	15	MOTA	4079	N	LEU A		28.478	58.203	93.185	1.00 22.92
	15	ATOM	4080	CA	LEU A		28.516	59.350	92.279	1.00 27.55
		MOTA	4081	C	LEU A		29.930	59.766	91.940	1.00 31.95
		ATOM	4082	0	LEU A		30.287	59.908	90.765	1.00 37.11
		ATOM	4083	CB	LEU A		27.673	60.564	92.741	1.00 30.03
	20	ATOM	4084 4085	CG	LEU A		27.428 26.648	61.626	91.648	1.00 32.87
20	20	ATOM ATOM	4086		LEU A		26.699	61.082 62.780	90.440 92.272	1.00 28.48 1.00 31.16
		ATOM	4087	N	GLY A		30.731	59.989	92.272	1.00 31.16
		ATOM	4088	CA	GLY A		32.131	60.384	92.811	1.00 25.59
		ATOM	4089	Ċ.	GLY A		32.902	59.472	91.835	1.00 23.33
	25	ATOM	4090	ŏ	GLY A		33.746	59.914	91.035	1.00 35.67
		ATOM	4091	N	HIS A		32.602	58.180	91.891	1.00 26.40
		ATOM	4092	CA	HIS A		33.257	57.255	90.998	1.00 25.86
25		ATOM	4093	С	HIS A		32.911	57.578	89.560	1.00 27.62
		ATOM	4094	0	HIS A		33.786	57.596	88.695	1.00 28.67
	30	ATOM	4095	CB	HIS A		32.826	55.814	91.282	1.00 25.39
		ATOM	4096	CG	HIS A	516	33.452	55.283	92.505	1.00 27.96
		ATOM	4097	ND1	HIS A	516	33.635	56.092	93.602	1.00 30.14
		ATOM	4098	CD2	HIS A	516	33.929	54.037	92.791	1.00 27.79
30		ATOM	4099	CE1	HIS A	516	34.205	55.336	94.534	1.00 27.58
30	35	ATOM	4100	NE2	HIS A		34.390	54.099	94.085	1.00 27.02
		ATOM	4101	N	ILE A		31.617	57.815	89.315	1.00 21.40
		MOTA	4102	CA	ILE A		31.137	58.107	87.973	1.00 22.75
		ATOM	4103	С	ILE A		31.706	59.424	87.462	1.00 31.09
	40	ATOM	4104	0	ILE A		32.246	59.558	86.352	1.00 28.78
	40	ATOM	4105	CB	ILE A		29.601	58.024	87.930	1.00 27.12
35		MOTA	4106		ILE A		29.225	56.610	88.312	1.00 29.40
		ATOM ATOM	4107 4108		ILE A		29.013 29.305	58.285 55.665	86.536	1.00 25.49
		ATOM	4109	N	ILE A LYS A		31.589	60.416	87.105 88.308	1.00 34.77 1.00 27.28
	45	ATOM	4110	CA	LYS A		32.108	61.690	87.955	1.00 27.28
	1.5	ATOM	4111	C	LYS A		33.558	61.482	87.485	1.00 24.03
		ATOM	4112	ŏ	LYS A		33.982	61.831	86.391	1.00 26.08
40		ATOM	4113	СВ	LYS A		32.038	62.557	89.210	1.00 24.00
40		ATOM	4114	CG	LYS A		30.641	63.060	89.591	1.00 19.24
	50	ATOM	4115	CD	LYS A		30.721	64.276	90.537	1.00 27.93
		ATOM	4116		LYS A		29.379		90.962	1.00 37.11
		ATOM	4117	NZ	LYS A	518	28.924	65.988	90.104	1.00 52.30
		ATOM	4118	N	ARG A		34.322	60.899	88.361	1.00 17.90
		ATOM	4119	CA	ARG A	519	35.703	60.636	88.098	1.00 20.80
45	55	ATOM	4120	С	ARG A	519	35.862	59.874	86.802	1.00 28.98
		ATOM	4121	0	ARG A	519	36.812	60.084	86.051	1.00 29.86
		ATOM	4122	СВ	ARG A	519	36.313	59.844	89.276	1.00 20.56
		ATOM	4123	CG	ARG A		37.721	59.308	89.036	1.00 29.02
		ATOM	4124	CD	ARG A	519	38.668	60.320	88.404	1.00 41.17
	60	ATOM	4125	NE	ARG A		40.086	60.008	88.616	1.00 59.84
50		ATOM	4126	CZ	ARG A		41.076	60.858	88.349	1.00 50.77
50		MOTA	4127		ARG A		40.838	62.073	87.880	1.00 31.21
		MOTA	4128		ARG A		42.329	60.486	88.543	1.00 31.86
		MOTA	4129	N	MET A	520	34.937	58.956	86.565	1.00 25.08

5		ATOM	4130	CA	MET A	520	34.979	58.121	85.379	1.00 24.56
		ATOM	4131	С	MET A	520	34.906	58.918	84.086	1.00 29.37
		ATOM	4132	0	MET A	520	35.651	58.687	83.114	1.00 27.92
	_	ATOM	4133	CB	MET A	520	33.905	57.007	85.442	1.00 26.98
	5	ATOM	4134	CG	MET A	520	34.082	55.902	84.399	1.00 28.02
		ATOM	4135	SD	MET A	520	32.830	54.591	84.479	1.00 27.87
		ATOM	4136	CE	MET A	520	33.246	53.825	86.070	1.00 22.09
10		ATOM	4137	N	GLN A		33.982	59.864	84.067	1.00 28.32
		ATOM	4138	CA	GLN A		33.838	60.672	82.886	1.00 28.34
	10	ATOM	4139	С	GLN A		35.067	61.540	82.785	1.00 36.52
		ATOM	4140	ō	GLN A		35.514	61.879	81.707	1.00 35.87
		ATOM	4141	СВ	GLN A		32.514	61.451	82.863	
		ATOM	4142	CG	GLN A		32.564	62.774	82.079	1.00 28.34
		ATOM	4143	CD	GLN A		32.890			1.00 9.68
15	15	ATOM	4144		GLN A		33.382	62.572	80.616	1.00 27.55
	10	ATOM	4145	NE2				63.491	79.924	1.00 28.25
		ATOM	4146	N			32.657	61.368	80.142	1.00 25.70
					GLU A		35.626	61.827	83.963	1.00 36.19
		ATOM	4147	CA	GLU A		36.818	62.648	84.171	1.00 36.13
	20	ATOM	4148	С	GLU A		38.136	62.046	83.662	1.00 42.48
	20	ATOM	4149	0	GLU A		39.099	62.735	83.335	1.00 42.40
20		ATOM	4150	CB	GLU A	522	36.857	63.035	85.641	1.00 37.79
20		ATOM	4151	CG	GLU A	522	38.233	63.196	86.273	1.00 58.85
		ATOM	4152	CD	GLU A	522	38.046	64.040	87.493	1.00 73.64
		ATOM	4153	OE1	GLU A	522	37.006	64.641	87.709	1.00 45.66
	25	ATOM	4154		GLU A		39.081	64.037	88.289	1.00 47.91
		ATOM	4155	N	VAL A		38.168	60.739	83.552	1.00 40.13
		ATOM	4156	CA	VAL A		39.401	60.136	83.058	
25		ATOM	4157	C	VAL A		39.205	59.351		1.00 37.49
25		ATOM	4158	õ	VAL A		40.195		81.778	1.00 38.88
	30	ATOM	4159	СВ	VAL A			59.016	81.138	1.00 40.21
	50	ATOM	4160				40.184	59.370	84.102	1.00 40.01
					VAL A		40.231	60.165	85.413	1.00 39.12
		ATOM	4161		VAL A		39.534	58.017	84.320	1.00 39.82
		ATOM	4162	N	TYR A		37.952	59.048	81.379	1.00 30.35
••	25	ATOM	4163	CA	TYR A		37.801	58.330	80.114	1.00 28.11
30	35	ATOM	4164	С	TYR A		37.061	59.144	79.074	1.00 33.14
		MOTA	4165	0	TYR A	524	37.076	58.802	77.908	1.00 35.84
		MOTA	4166	СВ	TYR A	524	37.281	56.878	80.119	1.00 25.56
		ATOM	4167	CG	TYR A	524	37.941	55.960	81.111	1.00 20.87
		ATOM	4168	CD1	TYR A	524	39.324	55.938	81.258	1.00 21.59
	40	ATOM	4169	CD2	TYR A	524	37.170	55.083	81.879	1.00 19.80
		ATOM	4170		TYR A		39.905	55.063	82.176	1.00 25.64
35		ATOM	4171	CE2			37.731	54.227	82.827	1.00 18.61
		MOTA	4172	CZ	TYR A		39.116	54.231	82.969	1.00 19.81
		ATOM	4173	OH	TYR A		39.706	53.402	83.863	
	45	ATOM	4174	N	ASN A		36.416	60.221	79.496	1.00 23.92
		ATOM	4175	CA	ASN A		35.687	61.088		1.00 25.98
		ATOM	4176	c.	ASN A		34.661		78.588	1.00 25.01
		ATOM	4177	ŏ	ASN A			60.354	77.735	1.00 29.86
40		ATOM	4178	СВ			34.533	60.535	76.499	1.00 29.39
	50	ATOM	4179		ASN A		36.637	61.922	77.739	1.00 29.55
	50			CG	ASN A		35.949	62.980	76.894	1.00 30.32
		ATOM	4180		ASN A		36.460	63.332	75.850	1.00 32.77
		ATOM	4181		ASN A		34.822	63.527	77.344	1.00 13.80
		MOTA	4182	N	PHE A		33.924	59.512	78.436	1.00 24.21
	<i></i>	MOTA	4183	CA	PHE A	526	32.900	58.745	77.807	1.00 25.14
45	55	MOTA	4184	С	PHE A	526	31.846	59.631	77.214	1.00 31.74
		ATOM	4185	0	PHE A	526	31.161	59.241	76.272	1.00 34.99
		ATOM	4186	CB	PHE A	526	32.256	57.732	78.781	1.00 26.60
		ATOM	4187	CG	PHE A		33.115	56.499	78.978	1.00 23.82
		ATOM	4188		PHE A		34.017	56.080	78.000	1.00 25.00
	60	MOTA	4189		PHE A		33.031	55.767		
		ATOM	4190		PHE A		34.783		80.159	1.00 21.74
50		ATOM	4191		PHE A		33.817	54.927	78.173	1.00 27.63
		ATOM	4192	CZ	PHE A			54.634	80.370	1.00 25.42
		ATOM	4192	N N			34.683	54.202	79.364	1.00 25.28
		WI OLI	7173	14	ASN A	321	31.689	60.815	77.760	1.00 28.22

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5		ATOM	4194	CA	ASN A	527	30.657	61.688	77.214	1.00 31.18
		MOTA	4195	c ·	ASN A		30.884	62.046	75.744	1.00 33.17
		ATOM	4196	0	ASN A		29.965	62.394	74.999	1.00 30.80
		ATOM	4197	СВ	ASN A		30.479	62.967	78.052	1.00 36.41
	5	ATOM	4198	CG	ASN A		29.638	62.752	79.292	1.00 46.99
		ATOM	4199	OD1	ASN A		29.647	63.571	80.209	1.00 36.82
		ATOM	4200		ASN A		28.922	61.636	79.338	1.00 30.02
10		ATOM	4201	N	ALA A		32.136	61.947	75.348	1.00 43.33
		ATOM	4202	CA	ALA A		32.581	62.278	74.005	
	10	ATOM	4203	c	ALA A		32.335	61.188	72.950	1.00 26.48
		ATOM	4204	ŏ	ALA A		32.420	61.404	71.753	1.00 32.09
		ATOM	4205	СВ	ALA A		34.076	62.584	74.105	1.00 32.09
		ATOM	4206	Й	ILE A		32.067	59.983		1.00 26.04
		ATOM	4207	CA	ILE A		31.854	58.859	73.402 72.529	1.00 31.35
15	15	ATOM	4208	Č.	ILE A					1.00 28.47
		ATOM	4209	ŏ	ILE A		30.492	58.904	71.887	1.00 35.96
		ATOM	4210	СВ	ILE A		29.486	59.023	72.578	1.00 38.79
		ATOM	4211				32.103	57.544	73.264	1.00 30.17
					ILE A		33.622	57.291	73.392	1.00 31.37
	20	ATOM	4212		ILE A		31.428	56.411	72.489	1.00 27.63
	20	ATOM '	4213		ILE A		34.059	56.515	74.635	1.00 33.41
20		ATOM	4214	N	ASN A		30.462	58.806	70.559	1.00 34.86
		ATOM	4215	CA	ASN A		29.196	58.841	69.852	1.00 36.44
	•	ATOM	4216	С	ASN A		28.596	57.495	69.473	1.00 39.90
	25	ATOM	4217	0	ASN A		27.452	57.437	69.043	1.00 41.37
	25	ATOM	4218	СВ	ASN A		28.951	60.044	68.928	1.00 51.44
		ATOM	4219	CG	ASN A	530	28.461	61.253	69.732	1.00100.00
		MOTA	4220		. ASN A		27.652	61.109	70.665	1.00100.00
25		MOTA	4221	ND2	ASN A	530	28.955	62.442	69.392	1.00 91.39
		MOTA	4222	N	ASN A	531	29.368	56.403	69.688	1.00 30.37
	30	ATOM	4223	CA	ASN A	531	28.912	55.030	69.446	1.00 28.14
		ATOM	4224	С	ASN A	531	27.696	54.753	70.360	1.00 32.80
		ATOM	4225	0	ASN A	531	27.746	54.887	71.611	1.00 36.74
		ATOM	4226	CB	ASN A	531	30.092	54.066	69.690	1.00 24.31
		ATOM	4227	CG	ASN A	531	29.770	52.601	69.730	1.00 34.44
30	35	ATOM	4228	OD1	ASN A		28.795	52.182	70.359	1.00 36.49
		ATOM	4229		ASN A		30.643	51.810	69.099	1.00 30.57
		ATOM	4230	N	SER A		26.570	54.403	69.734	1.00 22.02
		MOTA	4231	CA	SER A		25.325	54.183	70.459	1.00 19.67
		ATOM	4232	С	SER A		25.323	53.208	71.627	1.00 26.15
	40	ATOM	4233	0	SER A		24.767	53.475	72.680	1.00 26.64
		ATOM	4234	СВ	SER A		24.090	54.034	69.582	1.00 26.92
35		MOTA	4235	ŌĞ	SER A		24.294	53.211	68.452	
		ATOM	4236	N	GLU A		25.929	52.062	71.423	1.00 23.59
		ATOM	4237	CA	GLU A		25.995	51.036	72.420	1.00 22.68
	45	ATOM	4238	c.	GLU A		26.677			1.00 22.97
	••	MOTA	4239	ō	GLU A		26.125	51.569 51.539	73.635 74.749	1.00 30.48
		ATOM	4240	СВ	GLU A					1.00 31.13
		ATOM	4241	CG	GLU A		26.683 25.827	49.779	71.850	1.00 23.96
40		ATOM	4242	CD	GLU A			49.146	70.733	1.00 20.82
	50	ATOM	4243		GLU A		24.611	48.450	71.276	1.00 40.65
	20	ATOM	4244		GLU A	_	24.432	48.256	72.476	1.00 36.25
			4245				23.782	48.038	70.339	1.00 25.87
		ATOM		N	ILE A		27.872	52.101	73.392	1.00 26.20
		ATOM	4246	CA	ILE A		28.622	52.672	74.484	1.00 26.32
	55	ATOM	4247	C	ILE A		27.900	53.849	75.121	1.00 27.83
45	رو	ATOM	4248	0	ILE A		27.697	53.911	76.326	1.00 26.54
		ATOM	4249	CB	ILE A		30.051	53.022	74.102	1.00 29.16
	•	ATOM	4250		ILE A		30.738	51.808	73.479	1.00 29.47
		ATOM	4251		ILE A		30.801	53.458	75.353	1.00 28.28
	<i>(</i> 0	MOTA	4252	CD1	ILE A		32.038	52.184	72.765	1.00 34.99
	60	ATOM	4253	N	ARG A	535	27.480	54.805	74.320	1.00 24.30
		ATOM	4254	CA	ARG A	535	26.804	55.898	74.949	1.00 22.51
50		MOTA	4255	С	ARG A	535	25.573	55.401	75.701	1.00 28.19
		ATOM	4256	0	ARG A		25.212	55.808	76.791	1.00 32.61
		ATOM	4257	CB	ARG A		26.457	56.942	73.913	1.00 24.83
										21.03

5		MOTA	4258	CG	ARG A	535	25.970	58.229	74.541	1.00 21.49
		ATOM	4259	CD	ARG A		25.327	59.183	73.554	1.00 21.49
		MOTA	4260	NE	ARG A		25.194	60.457	74.213	1.00 31.38
		ATOM	4261	CZ	ARG A		26.256	61.140	74.554	1.00 29.41
	5	ATOM	4262	NH1	ARG A	535	27.463	60.677	74.259	1.00 26.45
		ATOM	4263	NH2	ARG A	535	26.110	62.302	75.195	1.00 19.99
40		ATOM	4264	N	PHE A	536	24.911	54.466	75.126	1.00 23.44
10		ATOM	4265	CA	PHE A	536	23.740	53.980	75.770	1.00 22.05
	10	MOTA	4266	С	PHE A		23.976	53.555	77.199	1.00 22.74
	10	ATOM	4267	0	PHE A		23.349	54.113	78.105	1.00 22.06
		MOTA	4268	CB	PHE A		23.117	52.865	74.919	1.00 23.17
		ATOM	4269	CG	PHE A		22.040	52.153	75.658	1.00 21.92
		ATOM	4270		PHE A		20.933	52.845	76.150	1.00 22.66
15	15	ATOM ATOM	4271 4272		PHE A		22.145	50.783	75.882	1.00 23.25
	10	ATOM	4273		PHE A		19.926	52.181	76.847	1.00 21.23
		ATOM	4274	CZ	PHE A		21.147	50.101	76.576	1.00 24.70
		ATOM	4275	N N	PHE A		20.047 24.863	50.811	77.065	1.00 20.57
		ATOM	4276	CA	ARG A		25.239	52.560 51.995	77.364	1.00 18.22
	20	ATOM	4277	c	ARG A		25.932	52.963	78.665 79.618	1.00 19.20
00		ATOM	4278	ŏ	ARG A		25.803	52.845	80.837	1.00 27.62
20		ATOM	4279	СВ	ARG A		26.035	50.709	78.556	1.00 26.73 1.00 18.91
		ATOM	4280	CG	ARG A		25.318	49.656	77.708	1.00 16.55
		ATOM	4281	CD	ARG A		26.181	48.426	77.387	1.00 21.58
	25	ATOM	4282	NE	ARG A		25.341	47.357	76.886	1.00 28.42
		MOTA	4283	CZ	ARG A		25.060	47.206	75.609	1.00 18.29
		ATOM	4284		ARG A		25.569	48.004	74.703	1.00 22.46
25		ATOM	4285		ARG A		24.240	46.236	75.224	1.00 25.22
		ATOM	4286	N	TRP A	538	26.668	53.930	79.064	1.00 24.21
	30	MOTA	4287	CA	TRP A	538	27.337	54.918	79.867	1.00 22.11
		MOTA	4288	С	TRP A	538	26.274	55.719	80.550	1.00 28.09
		MOTA	4289	0	TRP A	538	26.320	55.951	81,741	1.00 27.39
		ATOM	4290	СВ	TRP A		28.064	55.888	78.949	1.00 20.48
00	25	ATOM	4291	CG	TRP A		28.606	57.157	79.580	1.00 21.29
30	35	ATOM	4292		TRP A		28.641	58.345	78.968	1.00 22.86
		ATOM	4293		TRP A		29.286	57.352	80.845	1.00 21.79
		ATOM	4294		TRP A		29.228	59.270	79.769	1.00 22.70
		ATOM ATOM	4295 4296		TRP A		29.643	58.696	80.911	1.00 24.79
	40	ATOM	4297		TRP A		29.574	56.535	81.946	1.00 23.35
	70	ATOM	4298		TRP A		30.280	59.248	82.025	1.00 25.89
35		ATOM	4299		TRP A		30.203 30.562	57.056 58.405	83.046	1.00 23.35
		ATOM	4300	N	LEU A		25.303	56.161	83.081	1.00 24.89
		ATOM	4301	CA	LEU A		24.229	56.974	79.758 80.306	1.00 27.31
	45	ATOM	4302	c	LEU A		23.369	56.245	81.332	1.00 27.18 1.00 28.25
		ATOM	4303	ō	LEU A		22.857	56.822	82.266	1.00 27.19
		ATOM	4304	СВ	LEU A		23.428	57.812	79.262	1.00 26.37
40		ATOM	4305	CG	LEU A		24.269	58.682	78.279	1.00 25.71
40		ATOM	4306	CD1	LEU A		23.369	59.424	77.290	1.00 21.79
	50	ATOM	4307	CD2	LEU A	539	25.146	59.680	79.011	1.00 23.51
		ATOM	4308	N	ARG A	540	23.199	54.960	81.188	1.00 27.56
		ATOM	4309	CA	ARG A		22.390	54.283	82.170	1.00 26.88
		ATOM	4310	С	ARG A		23.145	54.229	83.453	1.00 31.82
	**	ATOM	4311	0	ARG A	540	22.618	54.448	84.539	1.00 32.72
45	55	ATOM	4312	CB	ARG A		22.034	52.888	81.732	1.00 24.48
		ATOM	4313	CG	ARG A		21.447	52.885	80.331	1.00 32.96
		ATOM	4314	CD	ARG A		20.695	51.597	80.090	1.00 33.19
		ATOM	4315	NE	ARG A		19.660	51.414	81.085	1.00 33.95
	60	ATOM	4316	CZ	ARG A		19.151	50.242	81.409	1.00 30.83
	60	ATOM	4317		ARG A		19.564	49.132	80.849	1.00 25.37
50		MOTA	4318		ARG A		18.186	50.186	82.317	1.00 30.30
50		MOTA	4319	N	LEU A		24.414	53.948	83.318	1.00 28.93
		ATOM	4320	CA	LEU A		25.239	53.895	84.505	1.00 26.36
		ATOM	4321	С	LEU A	341	25.036	55.210	85.277	1.00 31.00

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5		ATOM	4322	0	LEU A 541	24.632	55.246	86.439	1.00 31.62
		ATOM	4323	CB	LEU A 54:	26.702	53.586	84.094	1.00 23.61
		ATOM	4324	CG	LEU A 541	27.730	53.533	85.212	1.00 24.67
		ATOM	4325	CD1	LEU A 543		52.411	86.190	1.00 25.02
	5	ATOM	4326		LEU A 54		53.245	84.621	1.00 19.31
		ATOM	4327	N	CYS A 542		56.307	84.570	1.00 30.52
		ATOM	4328	CA	CYS A 542		57.661	85.105	
10		ATOM	4329	c	CYS A 542		57.996		1.00 31.76
		ATOM	4330	ŏ				85.805	1.00 32.71
	10	ATOM	4331		CYS A 542		58.536	86.914	1.00 33.97
	10			CB	CYS A 542		58.744	84.073	1.00 31.30
		ATOM	4332	SG	CYS A 542		58.488	83.347	1.00 34.39
		ATOM	4333	N	ILE A 543		57.708	85.125	1.00 25.61
		ATOM	4334	CA	ILE A 543		57.982	85.643	1.00 23.12
15	1.5	ATOM	4335	С	ILE A 543		57.161	86.885	1.00 30.15
, •	15	ATOM	4336	0	ILE A 543		57.645	87.972	1.00 30.73
		ATOM	4337	СВ	ILE A 543		57.627	84.585	1.00 23.75
		ATOM	4338	CG1	ILE A 543	20.369	58.664	83.468	1.00 24.09
		ATOM	4339	CG2	ILE A 543	18.955	57.572	85.182	1.00 22.99
		ATOM	4340	CD1	ILE A 543	20.386	60.109	83.982	1.00 27.34
	20	ATOM	4341	N	GLN A 544		55.884	86.695	1.00 27.99
00		ATOM	4342	CA	GLN A 54		54.929	87.756	1.00 25.72
20		ATOM	4343	C	GLN A 544		55.269	88.901	
		ATOM	4344	ō	GLN A 54		54.826		1.00 26.34
		ATOM	4345	СВ	GLN A 544			90.014	1.00 26.24
	25	ATOM	4346				53.512	87.210	1.00 26.76
	23			CG	GLN A 544		52.955	86.432	1.00 17.74
		ATOM	4347	CD	GLN A 544		51.604	85.743	1.00 32.62
		ATOM	4348		GLN A 544		51.432	84.551	1.00 38.66
25		ATOM	4349		GLN A 544		50.627	86.494	1.00 14.93
	20	ATOM	4350	N	SER A 545		56.033	88.625	1.00 21.73
	30	ATOM	4351	CA	SER A 545		56.392	89.685	1.00 22.42
		ATOM	4352	C	SER A 545	23.819	57.726	90.287	1.00 33.67
		MOTA	4353	0	SER A 545	24.567	58.257	91.133	1.00 37.22
		MOTA	4354	CB	SER A 545	25.646	56.322	89.338	1.00 21.57
		ATOM	4355	OG	SER A 545	25.980	54.968	89.163	1.00 31.72
30	35	ATOM	4356	N	LYS A 546		58.251	89.841	1.00 23.09
		ATOM	4357	CA	LYS A 546		59.490	90.356	1.00 20.79
		ATOM	4358	C	LYS A 546		60.738	89.961	1.00 27.55
		ATOM	4359	ō	LYS A 546		61.655	90.771	1.00 27.95
		ATOM	4360	СВ	LYS A 546		59.449	91.881	
	40	ATOM	4361	CG	LYS A 546				1.00 21.71
		ATOM	4362	CD	LYS A 546		58.195	92.484	1.00 15.90
35		ATOM	4363	CE			57.814	91.731	1.00 39.84
		ATOM	4364		LYS A 546		56.850	92.498	1.00 45.16
				NZ	LYS A 546		56.399	91.704	1.00 40.14
	45	ATOM	4365	N	TRP A 547		60.776	88.753	1.00 23.26
	43	ATOM	4366	CA	TRP A 547		61.931	88.289	1.00 21.90
		ATOM	4367	C	TRP A 547		62.901	87.570	1.00 29.82
		MOTA	4368	0	TRP A 547		62.679	86.432	1.00 34.91
40		ATOM	4369	СВ	TRP A 547		61.500	87.361	1.00 21.04
		ATOM	4370	CG	TRP A 547	26.254	62.591	87.206	1.00 22.57
	50	ATOM	4371	CD1	TRP A 547	26.224	63.769	87.844	1.00 25.87
		ATOM	4372	CD2	TRP A 547	27.437	62.588	86.417	1.00 23.40
		ATOM	4373	NE1	TRP A 547	27.316	64.511	87.517	1.00 25.64
		ATOM	4374		TRP A 547		63.819	86.635	1.00 27.46
		ATOM	4375		TRP A 547		61.668	85.547	1.00 26.21
45	55	ATOM	4376		TRP A 547		64.162	85.995	1.00 27.44
43		ATOM	4377		TRP A 547		62.009	84.923	1.00 28.70
		ATOM	4378		TRP A 547				
		ATOM	4379	N			63.236	85.138	1.00 28.41
		ATOM			GLU A 548		63.995	88.227	1.00 22.95
	60		4380	CA	GLU A 548		64.970	87.649	1.00 20.70
	00	ATOM	4381	C	GLU A 548		65.473	86.305	1.00 28.32
50		ATOM	4382	0	GLU A 548		65.735	85.391	1.00 29.41
50		ATOM	4383	CB	GLU A 548		66.144	88.607	1.00 22.45
		ATOM	4384	CG	GLU A 548		65.709	89.919	1.00 30.56
		ATOM	4385	CD	GLU A 548	20.337	66.848	90.765	1.00 59.35

5		MOTA	4386		GLU A 548	20.336	68.021	90.413	1.00 81.52
		MOTA	4387	OE2		19.888	66.450	91.925	1.00 57.05
		MOTA	4388	N	ASP A 549	23.728	65.661	86.201	1.00 24.72
	-	MOTA	4389	CA	ASP A 549	24.276	66.190	84.981	1.00 21.48
	5	ATOM	4390	С	ASP A 549	23.914	65.359	83.795	1.00 30.08
		MOTA	4391	0	ASP A 549	23.760	65.869	82.697	1.00 32.05
10		ATOM	4392	CB	ASP A 549	25.775	66.480	85.048	1.00 21.28
10		ATOM	4393	CG	ASP A 549	26.076	67.463	86.130	1.00 37.74
	10	MOTA	4394		ASP A 549	25.432	68.479	86.297	1.00 48.21
	10	MOTA	4395		ASP A 549	27.076	67.115	86.882	1.00 46.51
		MOTA	4396	N	ALA A 550	23.766	64.073	84.032	1.00 27.68
		MOTA ATOM	4397 4398	CA	ALA A 550	23.445	63.133	82.965	1.00 26.74
		ATOM	4399	0	ALA A 550 ALA A 550	22.019	63.171	82.431	1.00 32.35
15	15	ATOM	4400	СВ	ALA A 550	21.745 23.812	62.615 61.713	81.361	1.00 31.95
	13	ATOM	4401	N	ILE A 551	21.123	63.795	83.372	1.00 25.48
		ATOM	4402	CA	ILE A 551	19.716	63.882	83.192 82.832	1.00 28.71
		ATOM	4403	C	ILE A 551	19.461	64.355	81.411	1.00 28.20
		ATOM	4404	õ	ILE A 551	18.833	63.679	80.619	1.00 32.04 1.00 31.75
	20	MOTA	4405	СВ	ILE A 551	18.876	64.641	83.868	1.00 31.73
		ATOM	4406		ILE A 551	19.038	63.985	85.226	1.00 30.29
20		ATOM	4407		ILE A 551	17.391	64.661	83.475	1.00 24.75
		ATOM	4408		ILE A 551	18.072	64.561	86.253	1.00 24.73
		ATOM	4409	N	PRO A 552	19.969	65.529	81.099	1.00 33.75
	25	ATOM	4410	CA	PRO A 552	19.793	66.121	79.796	1.00 32.60
		ATOM	4411	С	PRO A 552	20.240	65.224	78.669	1.00 30.34
		ATOM	4412	0	PRO A 552	19.583	65.119	77.622	1.00 27.23
25		ATOM	4413	CB	PRO A 552	20.659	67.383	79.787	1.00 34.45
		MOTA	4414	CG	PRO A 552	21.348	67.500	81.139	1.00 38.39
	30	MOTA	4415	CD	PRO A 552	20.934	66.296	81.950	1.00 34.48
		ATOM	4416	N	LEU A 553	21.391	64.616	78.891	1.00 23.74
		MOTA	4417	CA	LEU A 553	21.997	63.727	77.931	1.00 22.72
		ATOM	4418	С	LEU A 553	21.138	62.522	77.670	1.00 32.68
	25	ATOM	4419	0	LEU A 553	21.015	62.087	76.523	1.00 35.70
30	35	ATOM	4420	CB	LEU A 553	23.362	63.281	78.439	1.00 21.57
		ATOM	4421	CG	LEU A 553	24.196	64.496	78.818	1.00 24.02
		ATOM	4422		LEU A 553	25.608	64.071	79.174	1.00 19.59
		MOTA	4423		LEU A 553	24.188	65.479	77.630	1.00 18.60
	40	ATOM	4424	N	ALA A 554	20.563	61.973	78.754	1.00 30.05
	70	ATOM ATOM	4425 4426	CA C	ALA A 554	19.726	60.779	78.669	1.00 27.72
35		ATOM	4427	0	ALA A 554 ALA A 554	18.432 17.944	61.107 60.332	77.988	1.00 36.03
		ATOM	4428	СВ	ALA A 554	19.475	60.332	77.163	1.00 37.08
		ATOM	4429	N	LEU A 555	17.898	62.283	80.017 78.320	1.00 26.78 1.00 29.70
	45	ATOM	4430	CA	LEU A 555	16.644	62.724	77.720	1.00 29.70
		ATOM	4431	c	LEU A 555	16.803	62.902	76.229	1.00 29.19
		ATOM	4432	ō	LEU A 555	15.970	62.506	75.385	1.00 26.13
40		ATOM	4433	СВ	LEU A 555	16.110	64.027	78.342	1.00 28.26
40		MOTA	4434	CG	LEU A 555	15.371	63.814	79.666	1.00 32.76
	50	ATOM	4435	CD1	LEU A 555	15.360	65.118	80.464	1.00 34.66
		ATOM	4436	CD2	LEU A 555	13.938	63.334	79.427	1.00 27.50
		MOTA	4437	N	LYS A 556	17.922	63.524	75.950	1.00 28.45
		ATOM	4438	CA	LYS A 556	18.325	63.839	74.615	1.00 28.76
		ATOM	4439	С	LYS A 556	18.369	62.591	73.800	1.00 35.11
45	55	MOTA	4440	0	LYS A 556	17.670	62.491	72.796	1.00 41.80
		ATOM	4441	СВ	LYS A 556	19.645	64.592	74.599	1.00 31.79
		ATOM	4442	CG	LYS A 556	20.101	65.139	73.250	1.00 63.55
		ATOM	4443	CD	LYS A 556	21.585	65.518	73.254	1.00 81.77
	40	MOTA	4444	CE	LYS A 556	22.046	66.270	72.011	1.00 79.68
	60	ATOM	4445	NZ	LYS A 556	23.239	65.661	71.401	1.00 73.00
50		ATOM	4446	N	MET A 557	19.154	61.623	74.248	1.00 26.96
50		ATOM	4447	CA	MET A 557	19.305	60.364	73.514	1.00 23.97
		ATOM	4448	C	MET A 557	18.033	59.553	73.287	1.00 30.96
		ATOM	4449	0	MET A 557	17.811	58.907	72.263	1.00 23.24

5		ATOM	4450	CB	MET A	557	20.401	59.488	74.104	1.00 24.89
		ATOM	4451	CG	MET A	557	20.533	58.163	73.368	1.00 29.37
		ATOM	4452	SD	MET A	557	22.029	57.276	73.864	1.00 33.21
	_	ATOM	4453	CE	MET A	557	21.939	55.812	72.793	1.00 30.16
	5	ATOM	4454	N	ALA A	558	17.203	59.568	74.287	1.00 33.42
		ATOM	4455	CA	ALA A	558	16.000	58.816	74.194	1.00 33.03
		ATOM	4456	С	ALA A	558	15.042	59.345	73.163	1.00 38.12
10		ATOM	4457	0	ALA A	558	14.349	58.568	72.543	1.00 37.09
	••	MOTA	4458	CB	ALA A	558	15.317	58.780	75.553	1.00 32.89
	10	ATOM	4459	N	THR A		14.994	60.665	73.032	1.00 36.76
		ATOM	4460	CA	THR A		14.067	61.326	72.144	1.00 36.43
		ATOM	4461	C	THR A		14.588	61.590	70.794	1.00 41.71
		ATOM	4462	0	THR A		13.788	61.768	69.891	1.00 44.66
15	15	ATOM	4463	CB	THR A		13.615	62.705	72.694	1.00 43.70
.•	15	ATOM	4464	0G1			14.728	63.545	72.957	1.00 38.88
		ATOM	4465	CG2			12.764	62.549	73.942	1.00 44.95
		ATOM	4466	N	GLU A		15.897	61.695	70.674	1.00 37.38
		ATOM	4467	CA	GLU A		16.495	62.018	69.395	1.00 36.51
	20	ATOM ATOM	4468 4469	C	GLU A		16.652	60.846	68.448	1.00 40.11
	20	ATOM	4470	O CB	GLU A		17.003	61.052	67.300	1.00 43.23
20		ATOM	4471	CG	GLU A		17.799	62.820	69.519	1.00 38.13
		ATOM	4472	CD	GLU A		17.653 18.857	64.142	70.292	1.00 54.29
		ATOM	4473	OE1			19.960	65.043 64.639	70.127	1.00 78.42
	25	ATOM	4474		GLU A		18.593	66.303	69.812	1.00 32.69
		ATOM	4475	N	GLN A		16.425	59.627	70.380 68.955	1.00 85.90
		ATOM	4476	CA	GLN A		16.467	58.356	68.230	1.00 30.45 1.00 22.57
25		ATOM	4477	c c	GLN A		15.398	57.523	68.878	1.00 26.95
25		ATOM	4478	ō	GLN A		14.978	57.814	69.975	1.00 27.79
	30	ATOM	4479	СВ	GLN A		17.829	57.661	68.128	1.00 20.64
		ATOM	4480	CG	GLN A		18.470	57.290	69.491	1.00 22.59
		ATOM	4481	CD	GLN A		17.802	56.121	70.184	1.00 28.22
		ATOM	4482	OE1	GLN A	561	17.524	56.156	71.400	1.00 37.44
		ATOM	4483	NE2	GLN A	561	17.556	55.069	69.419	1.00 31.92
30	35	ATOM	4484	N	GLY A	562	14.888	56.535	68.209	1.00 26.16
		ATOM	4485	CA	GLY A	562	13.801	55.810	68.858	1.00 27.83
		ATOM	4486	С	GLY A	562	13.932	54.320	68.761	1.00 41.56
		ATOM	4487	0	GLY A	562	12.936	53.614	68.677	1.00 45.37
	40	ATOM	4488	N	ARG A		15.171	53.864	68.742	1.00 37.40
	40	ATOM	4489	CA	ARG A		15.457	52.453	68.689	1.00 34.41
35		ATOM	4490	C	ARG A		15.121	51.939	70.109	1.00 39.48
55		ATOM	4491	0	ARG A		15.832	52.221	71.087	1.00 40.29
		ATOM	4492	CB	ARG A		16.932	52.231	68.284	1.00 18.23
	45	ATOM	4493	CG	ARG A		17.309	50.755	68.169	1.00 20.07
	40	ATOM ATOM	4494 4495	CD	ARG A		18.779	50.514	68.512	1.00 25.07
		ATOM	4496	NE CZ	ARG A		19.234	49.139	68.320	1.00 25.66
		ATOM	4497		ARG A		20.425	48.891	67.821	1.00 26.35
40		ATOM	4498		ARG A		21.257 20.804	49.860	67.430	1.00 12.96
	50	ATOM	4499	N	MET A		13.989	47.636 51.228	67.656	1.00 30.31
		ATOM	4500	CA	MET A		13.487	50.695	70.239 71.526	1.00 33.12
		ATOM	4501	c	MET A		14.565	50.247	72.532	1.00 31.84
		ATOM	4502	ŏ	MET A		14.494	50.501	73.744	1.00 31.42
		ATOM	4503	СВ	MET A		12.323	49.682	71.365	1.00 23.72
45	55	ATOM	4504	CG	MET A		11.196	50.225	70.487	1.00 35.78
73		ATOM	4505	SD	MET A		9.695	49.205	70.533	1.00 40.85
		ATOM	4506	CE	MET A		10.177	47.892	69.382	1.00 35.87
		ATOM	4507	N	LYS A		15.562	49.581	71.966	1.00 33.67
		ATOM	4508	CA	LYS A		16.699	49.041	72.668	1.00 29.04
	60	ATOM	4509	С	LYS A		17.281	50.089	73.562	1.00 26.36
		MOTA	4510	0	LYS A		. 17.648	49.782	74.673	1.00 21.19
50		ATOM	4511	CB	LYS A		17.747	48.494	71.697	1.00 29.06
		ATOM	4512	CG	LYS A	565	18.864	47.715	72.359	1.00 23.89
		ATOM	4513	CD	LYS A	565	19.982	47.355	71.392	1.00 35.75
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5		MOTA	4514	CE	LYS A	565	20.796	46.153	71.842	1.00 36.31
•		ATOM	4515	NZ	LYS A		22.233	46.311	71.577	1.00 36.31
		ATOM	4516	N	PHE A		17.321	51.321	73.073	1.00 22.91
		ATOM	4517	CA	PHE A		17.866	52.423	73.833	1.00 24.36
	5	ATOM	4518	С	PHE A		16.814	53.253	74.571	1.00 30.37
		ATOM	4519	0	PHE A		16.882	53.540	75.758	1.00 30.52
		ATOM	4520	CB	PHE A	566	18.622	53.355	72.857	1.00 25.26
10		ATOM	4521	CG	PHE A	566	19.738	52.677	72.088	1.00 24.09
		MOTA	4522	CD1	PHE A	566	20.392	51.559	72.609	1.00 23.51
	10	MOTA	4523	CD2	PHE A	566	20.165	53.187	70.858	1.00 24.48
		MOTA	4524		PHE A		21.432	50.958	71.900	1.00 23.73
		MOTA	4525		PHE A		21.211	52.620	70.129	1.00 24.75
		ATOM	4526	CZ	PHE A		21.828	51.491	70.668	1.00 25.20
15	15	ATOM	4527	N	THR A		15.860	53.679	73.801	1.00 31.17
,,	15	MOTA	4528	CA	THR A		14.783	54.533	74.239	1.00 31.74
		ATOM	4529	C	THR A		13.985	54.037	75.458	1.00 33.79
		ATOM	4530	0	THR A		13.657	54.818	76.373	1.00 26.01
		ATOM	4531 4532	CB	THR A		13.895	54.892	73.017	1.00 36.51
	20	ATOM	4533		THR A		14.527	55.844	72.138	1.00 24.12
	20	ATOM ATOM	4534				12.522	55.361	73.473	1.00 34.94
20		ATOM	4535	N CA	ARG A		13.663	52.726	75.469	1.00 30.74
		ATOM	4536	C	ARG A		12.864 13.486	52.166	76.545	1.00 26.30
		ATOM	4537	ŏ	ARG A		12.876	52.226	77.882	1.00 28.61
	25	ATOM	4538	СВ	ARG A		12.315	52.667 50.798	78.832	1.00 30.84
		ATOM	4539	CG	ARG A		11.342	50.730	76.251 75.088	1.00 18.11 1.00 29.19
		ATOM	4540	CD	ARG A		10.550	49.660	74.799	1.00 29.19
25		ATOM	4541	NE	ARG A		9.707	49.343	75.917	1.00 19.19
25		ATOM	4542	CZ	ARG A		9.254	48.138	76.133	1.00 32.39
	30	ATOM	4543		ARG A		9.528	47.144	75.291	1.00 32.39
		ATOM	4544		ARG A		8.507	47.930	77.208	1.00 16.44
		ATOM	4545	N	PRO A		14.705	51.774	77.925	1.00 28.41
		ATOM	4546	CA	PRO A		15.447	51.709	79.154	1.00 28.01
		ATOM	4547	С	PRO A	569	15.890	53.042	79.663	1.00 32.18
30	35	ATOM	4548	0	PRO A	569	15.974	53.256	80.869	1.00 29.25
		ATOM	4549	CB	PRO A	569	16.607	50.732	78.919	1.00 28.83
		ATOM	4550	CG	PRO A	569	16.330	50.034	77.592	1.00 32.42
		ATOM	4551	CD	PRO A		15.234	50.829	76.893	1.00 29.82
	40	ATOM	4552	N	LEU A		16.143	53.949	78.741	1.00 31.95
	40	ATOM	4553	CA	LEU A		16.560	55.270	79.160	1.00 35.11
35		ATOM	4554	C	LEU A		15.407	55.962	79.897	1.00 36.24
33		ATOM	4555	0	LEU A		15.532	56.506	81.028	1.00 34.02
		ATOM	4556	CB	LEU A		17.021	56.110	77.932	1.00 37.06
	45	ATOM ATOM	4557 4558	CG	LEU A		18.387	55.701	77.343	1.00 41.39
	43	ATOM	4559		LEU A		18.678	56.462	76.050	1.00 41.06
		ATOM	4560	N N	PHE A		19.497 14.262	55.984	78.353 79.211	1.00 37.42
		ATOM	4561	CA	PHE A		13.084	55.944 56.541		1.00 30.06
40		ATOM	4562	c	PHE A		12.813	55.899	79.758 81.095	1.00 27.27
	50	ATOM	4563	ŏ	PHE A		12.399	56.536	82.030	1.00 25.94 1.00 27.16
		ATOM	4564	СВ	PHE A		11.888	56.375	78.828	1.00 27.10
		ATOM	4565		PHE A		11.546	57.616	78.042	1.00 27.70
		ATOM	4566		PHE A		11.193	58.820	78.651	1.00 29.97
		ATOM	4567		PHE A		11.557	57.570	76.651	1.00 28.87
45	55	ATOM	4568		PHE A		10.861	59.953	77.910	1.00 28.24
70		ATOM	4569		PHE A		11.233	58.684	75.886	1.00 30.43
		ATOM	4570	CZ	PHE A		10.877	59.875	76.520	1.00 29.55
		ATOM	4571	N	LYS A		13.089	54.618	81.196	1.00 22.77
		ATOM	4572	CA	LYS A		12.845	53.946	82.468	1.00 25.43
	60	ATOM	4573	С	LYS A		13.783	54.425	83.561	1.00 34.48
		ATOM	4574	0	LYS A	572	13.351	54.920	84.602	1.00 35.11
50		ATOM	4575	CB	LYS A	572	12.736	52.428	82.392	1.00 26.89
		MOTA	4576	CG	LYS A		11.303	51.911	82.326	1.00 44.03
		ATOM	4577	CD	LYS A	572	11.219	50.426	81.922	1.00 57.87

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5		ATOM	4578	CE,	LYS A 572	10.975	50.204	80.422	1.00 65.25
		ATOM	4579	NZ	LYS A 572	11.535	48.954	79.850	1.00 61.06
		ATOM	4580	N	ASP A 573	15.074	54.292	83.319	1.00 31.94
	5	ATOM	4581	CA	ASP A 573	16.032	54.751	84.291	1.00 30.55
	כ	MOTA	4582	C	ASP A 573	15.684	56.166	84.712	1.00 32.26
		ATOM	4583	0	ASP A 573	15.693	56.453	85.895	1.00 31.85
10		MOTA	4584	CB	ASP A 573	17.453	54.788	83.718	1.00 32.87
,•		ATOM	4585	CG	ASP A 573	18.051	53.443	83.487	1.00 33.43
	10	MOTA MOTA	4586 4587		ASP A 573	17.517	52.422	83.853	1.00 29.11
	10	ATOM	4588	N	ASP A 573 LEU A 574	19.206	53.501	82.864	1.00 35.22
		ATOM	4589	CA	LEU A 574	15.387	57.071	83.745	1.00 29.50
		ATOM	4590	C	LEU A 574	15.062 13.887	58.461 58.577	84.109	1.00 27.65
		ATOM	4591	õ	LEU A 574	13.864	59.411	85,075 85,962	1.00 32.88
15	15	ATOM	4592	СВ	LEU A 574	14.844	59.385	82.909	1.00 31.04 1.00 26.24
	10	ATOM	4593	CG	LEU A 574	16.068	59.567	82.027	
		ATOM	4594		LEU A 574	15.644	59.922	80.582	1.00 30.41
		ATOM	4595		LEU A 574	16.974	60.659	82.604	1.00 27.06
		ATOM	4596	N	ALA A 575	12.895	57.723	84.874	1.00 32.80
	20	ATOM	4597	CA	ALA A 575	11.709	57.713	85.711	1.00 32.00
••		ATOM	4598	c .	ALA A 575	12.002	57.140	87.083	1.00 35.71
20		ATOM	4599	ō	ALA A 575	11.309	57.362	88.055	1.00 39.91
		ATOM	4600	ĊВ	ALA A 575	10.631	56.890	85.024	1.00 30.56
		ATOM	4601	N	ALA A 576	13.049	56.364	87.170	1.00 28.55
	25	ATOM	4602	CA	ALA A 576	13.390	55.778	88.448	1.00 22.80
		ATOM	4603	С	ALA A 576	14.258	56.724	89.266	1.00 26.93
		ATOM	4604	0	ALA A 576	14.444	56.591	90.461	1.00 30.45
25		ATOM	4605	CB	ALA A 576	14.023	54.415	88.245	1.00 20.31
		ATOM	4606	N	PHE A 577	14.787	57.686	88.584	1.00 22.86
	30	ATOM	4607	CA	PHE A 577	15.604	58.673	89.194	1.00 22.71
		ATOM	4608	С	PHE A 577	14.651	59.751	89.673	1.00 32.25
		ATOM	4609	0	PHE A 577	13.930	60.334	88.863	1.00 34.17
		ATOM	4610	СВ	PHE A 577	16.640	59.188	88.154	1.00 22.89
		MOTA	4611	CG	PHE A 577	17.704	60.076	88.741	1.00 23.16
30	35	· ATOM	4612	CD1	PHE A 577	17.847	60.231	90.120	1.00 26.60
		ATOM	4613		PHE A 577	18.561	60.806	87.914	1.00 23.46
		ATOM	4614		PHE A 577	18.818	61.082	90.661	1.00 27.55
		ATOM	4615		PHE A 577	19.543	61.657	88.431	1.00 23.88
	40	ATOM	4616	CZ	PHE A 577	19.669	61.791	89.813	1.00 23.59
	40	ATOM	4617	N	ASP A 578	14.625	60.008	90.990	1.00 29.70
35		ATOM	4618	CA	ASP A 578	13.717	61.018	91.533	1.00 28.65
30		ATOM	4619	С	ASP A 578	13.862	62.357	90.881	1.00 28.55
		ATOM	4620	0	ASP A 578	12.877	63.004	90.599	1.00 32.65
	45	ATOM	4621	CB	ASP A 578	13.804	61.192	93.055	1.00 32.60
	43	ATOM	4622	CG	ASP A 578	15.153	61.647	93.550	1.00 53.21
		ATOM ATOM	4623 4624		ASP A 578	16.175	61.594	92.872	1.00 51.81
			4625		ASP A 578	15.104	62.072	94.796	1.00 64.93
40		ATOM ATOM	4625	N CA	LYS A 579 LYS A 579	15.104 15.470	62.750	90.674	1.00 20.12
	50	ATOM	4627	C	LYS A 579		64.012	90.084	1.00 21.01
	50	ATOM	4628	0	LYS A 579	14.934 14.620	64.270	88.697	1.00 30.25
		ATOM	4629	СВ	LYS A 579	16.982	65.413 64.223	88.368 90.104	1.00 35.12
		ATOM	4630	CG	LYS A 579	17.552	64.202	91.512	1.00 24.11 1.00 48.98
		ATOM	4631	CD	LYS A 579	17.252	65.488	92.286	1.00 46.96
45	55	ATOM	4632	CE	LYS A 579	16.495	65.258	93.588	1.00 76.92
43		ATOM	4633	NZ	LYS A 579	17.282	64.550	94.611	1.00 89.56
		ATOM	4634	N	SER A 580	14.838	63.244	87.857	1.00 28.66
		ATOM	4635	CA	SER A 580	14.368	63.437	86.459	1.00 28.56
		ATOM	4636	C	SER A 580	13.007	62.829	86.129	1.00 32.95
	60	ATOM	4637	ō	SER A 580	12.561	62.870	84.992	1.00 35.30
		MOTA	4638	СВ	SER A 580	15.337	62.774	85.517	1.00 25.69
50		MOTA	4639	OG	SER A 580	15.476	61.424	85.969	1.00 25.12
		MOTA	4640	N	HIS A 581	12.364	62.230	87.098	1.00 26.81
		ATOM	4641	CA	HIS A 581	11.100	61.595	86.850	1.00 28.26

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5		ATOM	4642	C ,	HIS			10.067	62.399	86.042	1.00 36.50
		ATOM	4643	0	HIS			9.644	62.031	84.927	1.00 34.71
		ATOM	4644	CB	HIS			10.553	61.047	88.152	1.00 29.76
	5	ATOM	4645	CG	HIS			9.148	60.588	87.968	1.00 35.31
	3	ATOM	4646		HIS			8.111	61.494	87.899	1.00 38.92
		ATOM	4647		HIS			8.634	59.338	87.891	1.00 36.84
10		MOTA MOTA	4648 4649		HIS			6.999	60.783	87.817	1.00 38.85
		ATOM	4650	N	ASP			7.280	59.488	87.734	1.00 38.13
	10	ATOM	4651	CA	ASP			9.656 8.680	63.502 64.388	86.639	1.00 35.79
	10	ATOM	4652	Č	ASP			9.035	64.807	86.064 84.659	1.00 34.39 1.00 37.82
		ATOM	4653	ō	ASP			8,220	64.704	83.735	1.00 37.01
		ATOM	4654	CB	ASP			8.428	65.552	87.001	1.00 36.57
		ATOM	4655	CG	ASP			7.597	65.110	88.167	1.00 58.09
15	15	ATOM	4656		ASP			6.708	64.289	88.070	1.00 63.17
		MOTA	4657		ASP			7.920	65.708	89.279	1.00 73.96
		MOTA	4658	N	GLN			10.272	65.255	84.488	1.00 32.88
		MOTA	4659	CA	GLN	Α.	583	10.750	65.648	83.169	1.00 29.92
		MOTA	4660	С	GLN	A :	583	10.690	64.464	82.168	1.00 37.12
	20	MOTA	4661	0	GLN	A	583	10.362	64.624	80.990	1.00 37.42
20		MOTA	4662	CB	GLN	A	583	12.172	66.182	83.287	1.00 28.54
20		ATOM	4663	CG	GLN	A.	583	12.704	66.648	81.929	1.00 48.12
		MOTA	4664	CD	GLN			13.957	67.475	82.081	1.00 64.09
	0.0	ATOM	4665		GLN			14.736	67.248	83.015	1.00 59.43
	25	MOTA	4666		GLN			14.130	68.461	81.201	1.00 55.34
		ATOM	4667	N	ALA			11.009	63.250	82.638	1.00 33.22
		MOTA	4668	CA	ALA			10.964	62.062	81.780	1.00 32.22
25		ATOM	4669	C	ALA			9.557	61.841	81.315	1.00 37.45
	20	MOTA	4670	0	ALA			9.319	61.526	80.152	1.00 40.05
	30	ATOM	4671	СВ	ALA			11.389	60.793	82.504	1.00 31.62
		ATOM	4672	N	VAL			8.622	61.995	82.261	1.00 30.42
		ATOM	4673	CA	VAL			7.217	61.806	81.946	1.00 29.16
		ATOM ATOM	4674 4675	С 0	VAL			6.647	62.909	81.024	1.00 36.53
30	35	ATOM	4676	СВ	VAL VAL			5.933 6.408	62.690	80.052	1.00 36.22
30	33	ATOM	4677		VAL			4.959	61.567 61.947	83.209 82.955	1.00 29.78 1.00 30.03
		ATOM	4678		VAL			6.464	60.085	83.539	1.00 30.03
		ATOM	4679	N	ARG			7.000	64.123	81.333	1.00 27.82
		ATOM	4680	CA	ARG			6.574	65.242	80.562	1.00 36.20
	40	ATOM	4681	С	ARG			7.146	65.125	79.180	1.00 44.65
Ω		MOTA	4682	0	ARG			6.459	65.355	78.197	1.00 48.32
35		MOTA	4683	СВ	ARG			7.116	66.498	81.208	1.00 38.13
		MOTA	4684	CG	ARG	A	586	6.744	67.799	80.518	1.00 61.01
		MOTA	4685	CD	ARG	A :	586	7.077	69.029	81.354	1.00 73.03
	45	ATOM	4686	NE	ARG	A	586	8.491	69.128	81.711	1.00 86.05
		MOTA	4687	CZ	ARG	A	586	8.961	69.001	82.957	1.00 98.46
		MOTA	4688		ARG			8.167	68.741	84.004	1.00 79.75
40		ATOM	4689	NH2	ARG			10.268	69.103	83.159	1.00 77.55
, ,	50	ATOM	4690	N	THR			8.426	64.769	79.110	1.00 39.49
	50	ATOM	4691	CA	THR			9.099	64.646	77.822	1.00 36.80
		ATOM	4692	C	THR			8.387	63.690	76.869	1.00 37.11
		ATOM	4693	0	THR			8.229	63.931	75.678	1.00 36.91
		MOTA	4694	CB	THR	A	587	10.634	64.384	77.917	1.00 39.40
	55	ATOM	4695		THR			11.303	65.334	78.717	1.00 46.27
45	22	MOTA	4696		THR			11.233	64.460	76.529	1.00 32.60
		MOTA	4697 4698	N	TYR			7.934	62.587	77.393	1.00 33.33
		ATOM ATOM	4699	CA C	TYR			7.252	61.639	76.555	1.00 33.94
		ATOM	4700	0	TYR TYR			5.890 5.428	62.146	76.090	1.00 37.02
	60	ATOM	4701	СВ	TYR			5.428 7.042	61.880	74.988	1.00 41.55
	· ·	ATOM	4702	CG	TYR			6.017	60.383	77.396	1.00 33.96
50		ATOM	4703		TYR			6.331	59.440	76.851	1.00 33.08
		ATOM	4704		TYR			4.758	58.640	75.754	1.00 35.64
		ATOM	4705		TYR			5.424	59.288 57.703	77.437 75.251	1.00 34.09
		011	1,00		- 11		200	3.424	21.103	13.231	1.00 34.36

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		ATOM	4706	CE2	TYR A 588	3.822	58.378	76.932	1.00 34.05
		ATOM	4707	CZ	TYR A 588	4.162	57.581	75.834	1.00 33.89
		ATOM	4708	ОН	TYR A 588	3.275	56.674	75.322	1.00 23.43
		ATOM	4709	N	GLN A 589	5.216	62.853	76.959	1.00 25.04
	5	ATOM	4710	CA	GLN A 589	3.914	63.339	76.612	1.00 21.41
10		ATOM	4711	С	GLN A 589	3.992	64.304	75.481	1.00 28.78
		ATOM	4712	0	GLN A 589	3.099	64.410	74.678	1.00 31.24
		ATOM	4713	СВ	GLN A 589	3.241	63.935	77.832	1.00 21.73
	10	ATOM	4714	CG	GLN A 589	2.878	62.820	78.827	1.00 22.30
	10	ATOM	4715	CD	GLN A 589	1.695	62.069	78.293	1.00 52.83
		MOTA	4716		GLN A 589	1.511 0.864	62.003 61.542	77.075 79.182	1.00 60.15 1.00 53.04
15		ATOM ATOM	4717 4718	NEZ N	GLN A 589 GLU A 590	5.099	65.001	75.409	1.00 28.36
15		ATOM	4719	CA	GLU A 590	5.276	65.966	74.355	1.00 26.87
	15	ATOM	4720	c .	GLU A 590	5.840	65.338	73,140	1.00 35.10
		ATOM	4721	Ō	GLU A 590	6.096	66.059	72.171	1.00 40.28
		ATOM	4722	CB	GLU A 590	6.323	67.011	74.747	1.00 27.61
		ATOM	4723	CG	GLU A 590	5.846	67.954	75.847	1.00 44.11
0.2		ATOM	4724	CD	GLU A 590	6.981	68.759	76.388	1.00 75.35
20	20	ATOM	4725		GLU A 590	8.120	68.689	75.925	1.00 54.78
		ATOM	4726		GLU A 590	6.609	69.516	77.403	1.00 59.46
		ATOM	4727	N	HIS A 591	6.091	64.031	73.207	1.00 27.57
		ATOM	4728	CA	HIS A 591	6.713	63.384	72.086 71.578	1.00 25.58
	25	ATOM	4729 4730	C	HIS A 591	5.928 6.184	62.249 61.751	70.496	1.00 32.34 1.00 38.53
	23	ATOM ATOM	4730	O CB	HIS A 591 HIS A 591	8.094	62.851	72.487	1.00 26.32
25		MOTA	4732	CG	HIS A 591	9.219	63.809	72.268	1.00 31.06
		ATOM	4733		HIS A 591	9.630	64.680	73.255	1.00 32.65
		ATOM	4734		HIS A 591	9,998	64.032	71.169	1.00 34.91
	30	ATOM	4735		HIS A 591	10.635	65.404	72.756	1.00 32.01
		ATOM	4736	NE2	HIS A 591	10.884	65.037	71.508	1.00 33.36
		ATOM	4737	N	LYS A 592	4.978	61.812	72.337	1.00 28.34
30		ATOM	4738	CA	LYS A 592	4.254	60.643	71.849	1.00 29.96
	0.5	MOTA	4739	С	LYS A 592	3.654	60.692	70.432	1.00 33.41
	35	ATOM	4740	0	LYS A 592	3.819	59.769	69.592	1.00 29.05
		ATOM	4741	CB	LYS A 592	3.362 2.435	59.983 60.930	72.888 73.615	1.00 32.83 1.00 31.14
		ATOM ATOM	4742 4743	CD	LYS A 592 LYS A 592	1.677	60.203	74.704	1.00 38.97
		ATOM	4744	CE	LYS A 592	0.253	60.691	74.890	1.00 25.02
35	40	ATOM	4745	NZ	LYS A 592	-0.157	60.632	76.302	1.00 45.83
50		ATOM	4746	N	ALA A 593	2.934	61.782	70.187	1.00 30.97
		ATOM	4747	CA	ALA A 593	2.260	62.026	68.917	1.00 28.47
		ATOM	4748	С	ALA A 593	3.169	61.943	67.703	1.00 32.66
	4.5	MOTA	4749	0	ALA A 593	2.775	61.488	66.639	1.00 36.77
	45	ATOM	4750	СВ	ALA A 593	1.571	63.379	68.954	1.00 27.35
40		MOTA	4751	N	SER A 594	4.384	62.405	67.869	1.00 27.08
40		MOTA MOTA	4752 4753	CA C	SER A 594 SER A 594	5.345 6.185	62.417 61.169	66.794 66.760	1.00 30.04 1.00 36.80
		MOTA	4754	ŏ	SER A 594	6.995	60.991	65.848	1.00 37.94
	50	ATOM	4755			6.292	63.596		1.00 37.69
	••	ATOM	4756	OG	SER A 594	7.199	63.340	68.043	1.00 54.55
		MOTA	4757	N	MET A 595	6.015	60.340	67.776	1.00 33.12
45		MOTA	4758	CA	MET A 595	6.794	59.115	67.898	1.00 33.96
45		ATOM	4759	С	MET A 595	6.200	57.936	67.125	1.00 40.91
	55	MOTA	4760	0	MET A 595	5.019	57.927	66.809	1.00 50.82
		ATOM	4761	CB	MET A 595	6.716	58.686	69.382	1.00 34.22
		ATOM	4762	CG	MET A 595	7.621	59.371	70.399	1.00 34.61
		ATOM	4763.	SD	MET A 595	7.606	58.440	71.962	1.00 39.24
	60	ATOM	4764 4765	CE	MET A 595	7.145 6.987	59.779 56.897	73.084 66.886	1.00 36.72 1.00 26.19
50	UU	ATOM ATOM	4765	N CA	HIS A 596 HIS A 596	6.496	55.657	66.246	1.00 23.19
		ATOM	4767	c	HIS A 596	5.438	54.964	67.120	1.00 25.21
		ATOM	4768	ŏ	HIS A 596	5.621	54.728	68.311	1.00 22.59
		MOTA	4769	СВ	HIS A 596	7.657	54.655	66.077	1.00 24.41

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5		ATOM	4770		HIS A		7.222	53.366	65.493	1.00 30.13
		ATOM	4771		HIS A		7.606	52.995	64.214	1.00 32.86
		ATOM	4772		HIS A		6.421	52.385	66.005	1.00 30.90
	5	ATOM	4773		HIS A		7.047	51.824	63.974	1.00 30.05
	5	ATOM	4774		HIS A		6.325	51.441	65.031	1.00 30.20
		ATOM	4775	N	PRO A		4.334	54.587	66.512	1.00 27.08
10		MOTA	4776	CA	PRO A		3.217	53.912	67.173	1.00 26.35
10		ATOM	4777	C	PRO A		3.513	52.851	68.248	1.00 37.51
	10	ATOM	4778	0	PRO A		2.979	52.900	69.348	1.00 41.16
	10	ATOM	4779	CB	PRO A		2.334	53.307	66.076	1.00 26.17
		ATOM	4780	CG	PRO A		3.140	53.426	64.792	1.00 34.56
		MOTA	4781	CD	PRO A		4.285	54.418	65.050	1.00 30.06
		ATOM	4782	Ņ	VAL A		4.311	51.850	67.939	1.00 33.08
15	15	ATOM	4783	CA	VAL A		4.585	50.802	68.911	1.00 28.39
	13	ATOM	4784	C	VAL A		5.444	51.307	70.029	1.00 29.32
		ATOM	4785	0	VAL A		5.168	51.096	71.217	1.00 29.13
		ATOM	4786	CB	VAL A		5.196	49.599	68.210	1.00 27.99
		ATOM	4787		VAL A		5.806	48.608	69.187	1.00 26.98
	20	ATOM	4788		VAL A		4.144	48.944	67.296	1.00 26.13
	20	ATOM	4789	N	THR A		6.480	52.021	69.635	1.00 26.10
20		ATOM	4790	CA	THR A		7.370	52.573	70.631	1.00 26.95
		ATOM	4791	С	THR A		6.650	53.404	71.669	1.00 30.81
		ATOM	4792	0	THR A		6.863	53.327	72.871	1.00 31.33
	25	ATOM	4793	CB	THR A		8.413	53.455	69.975	1.00 26.67
	25	ATOM	4794		THR A		9.092	52.725	68.958	1.00 27.92
		ATOM	4795		THR A		9.358	53.884	71.092	1.00 20.69
		ATOM	4796	N	ALA A		5.801	54.218	71.135	1.00 26.41
25		ATOM	4797	CA	ALA A		4.997	55.111	71.878	1.00 26.39
	20	ATOM	4798	C	ALA A		4.176	54.339	72.860	1.00 32.00
	30	ATOM	4799	0	ALA A		4.162	54.597	74.057	1.00 35.37
		ATOM	4800	CB	ALA A		4.090	55.774	70.856	1.00 27.56
		ATOM	4801	N	MET A		3.470	53.380	72.332	1.00 26.26
		ATOM	4802	CA	MET A		2.627	52.585	73.167	1.00 26.60
	25	MOTA	4803	C	MET A		3.439	51.909	74.225	1.00 25.73
30	35	ATOM	4804	0	MET A		3.099	51.964	75.381	1.00 25.77
		ATOM	4805	СВ	MET A		1.752	51.625	72.353	1.00 30.49
		ATOM	4806	CG	MET A		1.024	50.594	73.176	1.00 36.00
		ATOM	4807	SD	MET A		2.043	49.146	73.554	1.00 42.41
	40	ATOM	4808	CE	MET A		1.693	48.128	72.111	1.00 37.75
	40	ATOM	4809	N	LEU A		4.538	51.310	73.848	1.00 21.64
35		ATOM	4810	CA	LEU A		5.339	50.671	74.873	1.00 22.59
33		ATOM	4811	С	LEU A		6.010	51.650	75.870	1.00 29.61
		ATOM	4812	0	LEU A		6.137	51.346	77.039	1.00 27.62
	45	ATOM	4813	CB	LEU A		6.418	49.760	74.294	1.00 22.14
	43	ATOM	4814	CG	LEU A		5.916	48.529	73.575	1.00 25.78
		ATOM	4815		LEU A		7.021	48.087	72.609	1.00 26.02
		ATOM	4816		LEU A		5.651	47.445	74.613	1.00 21.01
40		ATOM	4817	N	VAL A		6.508	52.805	75.445	1.00 27.15
	50	ATOM	4818	CA	VAL A		7.145	53.684	76.413	1.00 26.39
	30	ATOM	4819	C	VAL A		6.121	54.157	77.438	1.00 32.60
		ATOM	4820	0	VAL A		6.436	54.235	78.621	1.00 35.31
		ATOM	4821	CB	VAL A		7.917	54.832	75.760	1.00 27.78
		ATOM	4822		VAL A		8.286	55.887	76:774	1.00 24.54
	55	ATOM	4823		VAL A		9.172	54.286	75.094	1.00 27.29
45	22	ATOM	4824	N	GLY A		4.878	54.434	76.976	1.00 27.44
		ATOM	4825	CA	GLY A		3.759	54.856	77.819	1.00 27.58
		ATOM	4826	C	GLY A		3.418	53.797	78.905	1.00 37.00
		ATOM	4827	0	GLY A		3.088	54.102	80.072	1.00 36.56
	60	ATOM	4828	N	LYS A		3.511	52.522	78.520	1.00 32.54
	60	ATOM	4829	CA	LYS A		3.250	51.415	79.459	1.00 32.17
50		ATOM	4830	C	LYS A		4.312	51.405	80.539	1.00 35.15
50		ATOM	4831	0	LYS A		4.040	51.347	81.734	1.00 33.77
		ATOM	4832	CB	LYS A		3.231	50.034	78.782	1.00 33.59
		ATOM	4833	CG	LYS A	605	1.837	49.438	78.576	1.00 42.45

5		ATOM	4834	CD.	LYS A	605	1.846	48.115	77.815	1.00 60.83
		ATOM	4835	CE	LYS A	605	1.223	46.946	78.578	1.00 86.38
		ATOM	4836	NZ	LYS A	605	2.188	46.179	79.385	1.00 93.05
		ATOM	4837	N	ASP A	4 606	5.544	51.470	80.056	1.00 32.91
	5	MOTA	4838	CA	ASP A	606	6.715	51.510	80.878	1.00 31.82
		ATOM	4839	С	ASP A	606	6.549	52.667	81.833	1.00 36.24
40		ATOM	4840	0	ASP A	4 606	6.652	52.503	83.045	1.00 35.19
10		ATOM	4841	CB	ASP A	606	7.983	51.702	80.027	1.00 32.52
		ATOM	4842	CG	ASP A	606	8.302	50.525	79.134	1.00 40.01
	10	ATOM	4843	OD1	ASP A		7.934	49.378	79.344	1.00 40.49
		ATOM	4844	OD2	ASP A	4 606	9.038	50.869	78.111	1.00 41.73
		ATOM	4845	N	LEU A		6.240	53.833	81.266	1.00 34.45
		ATOM	4846	CA	LEU A		6.152	54.972	82.185	1.00 36.03
15		ATOM	4847	С	LEU A		4.814	55.018	82.968	1.00 42.35
15	15	ATOM	4848	0	LEU A		4.600	55.872	83.824	1.00 41.57
		ATOM	4849	CB	LEU A		6.321	56.250	81.364	1.00 36.90
		ATOM	4850	CG	LEU A		7.779	56.490	80.974	1.00 38.75
		ATOM	4851		LEU A		7.954	57.746	80.132	1.00 34.34
		ATOM	4852		LEU A		8.695	56.653	82.183	1.00 41.97
	20	ATOM	4853	N	LYS A		3.895	54.062	82.586	1.00 45.01
20		ATOM	4854	CA	LYS A		2.576	53.874	83.264	1.00 46.99
20		ATOM	4855	c c	LYS A		1.625	55.088	83.181	1.00 51.31
		ATOM	4856	ō	LYS A		0.988	55.467	84.151	
		ATOM	4857	СВ	LYS A		2.813	53.510	84.750	1.00 51.35
	25	ATOM	4858	CG	LYS A		3.331	52.093		1.00 50.83
	23	ATOM	4859		LYS F				84.949	1.00 63.57
		ATOM		CD			4.405	52.019	86.031	1.00 77.03
25			4860	CE	LYS A		5.341	50.825	85.858	1.00 96.40
25		ATOM	4861	NZ	LYS A		6.034	50.554	87.117	1.00100.00
	30	ATOM	4862	N	VAL A		1.560	55.724	81.991	1.00 50.28
	30	ATOM	4863	CA	VAL A		0.688	56.901	81.852	1.00 50.89
		ATOM	4864	C	VAL A		-0.494	56.660	80.897	1.00 60.23
		ATOM	4865	0	VAL A		-1.640	56.952	81.194	1.00 63.02
		MOTA	4866	CB	VAL A		1.533	58.091	81.364	1.00 54.72
30	25	ATOM	4867		VAL A		1.996	58.926	82.551	1.00 54.87
30	35	ATOM	4868		VAL A		2.744	57.607	80.605	1.00 54.46
		ATOM	4869	N	ASP A		-0.177	56.152	79.687	1.00 58.84
		ATOM	4870	CA.	ASP A		-1.238	55.949	78.699	1.00 99.84
		ATOM	4871	С	ASP A		-2.062	54.695	79.001	1.00100.00
	40	ATOM	4872	0	ASP A		-3.247	54.615	78.711	1.00 69.75
	40	ATOM	4873	CB	ASP A		-0.594	55.818	77.316	1.00100.00
35		ATOM	4874	CG	ASP F		-0.637	57.161	76.610	1.00 92.61
		ATOM	4875		ASP A		-1.449	57.999	77.018	1.00 90.49
		MOTA	4876		ASP A		0.134	57.355	75.670	1.00 89.29
	4.0	ATOM		ZN2+			17.003	38.803	64.180	1.00 28.37
	45	MOTA		YB3+			43.011	51.068	98.864	1.00 34.70
		MOTA		YB3+			-13.786	56.771	52.040	0.50 57.25
		ATOM		YB3+			-10.537	57.860	52.381	0.50 36.57
40		ATOM	4881	CG	IMD 1		26.249	42.039	80.754	1.00 28.44
	**	ATOM	4882	ND1	IMD]	1	26.057	42.254	79.400	1.00 28.35
	50	ATOM	4883	CD2	IMD 1	1	27.562	41.726	80.902	1.00 17.99
		ATOM	4884		IMD 1		27.201	42.063	78.760	1.00 29.77
		ATOM	4885	NE2	IMD]	1	28.130	41.745	79.647	1.00 35.02
		ATOM	4886	CB	ACE (1	13.616	12.333	68.475	1.00 59.33
		ATOM	4887	CG	ACE (1	12.871	13.331	69.306	1.00 42.98
45	55	ATOM	4888	OD1	ACE (12.958	14.536	69.146	1.00 39.66
		ATOM	4889		ACE (12.142	12.759	70.236	1.00 47.21
		ATOM	4890	С6	INH V		7.422	38.514	70.154	1.00 38.70
		ATOM	4891	C5	INH V		7.571	39.820	69.689	1.00 37.05
		ATOM	4892	C4	INH V		7.901	40.062	68.354	1.00 31.41
	60	ATOM	4893	C3	INH V		8.091	38.967	67.505	1.00 35.48
	- *	ATOM	4894	C2	INH V		7.944	37.650	67.949	1.00 31.90
50		ATOM	4895	C1	INH V		7.611	37.434	69.286	1.00 36.93
		ATOM	4896	c7	INH		8.071	41.463	67.833	1.00 32.28
		ATOM	4897	01	INH V		8.288	41.443	66.485	1.00 37.06
			.551	J 1			0.200	21.443	00.400	2.00 37.00

5										
•		ATOM	4898	C8	INH V	1	9.584	41.740	66.129	1.00 32.34
		ATOM	4899	C9	INH V	1	9.825	42.911	65.416	1.00 31.03
		MOTA	4900		INH V	1	11.127	43.216	65.023	1.00 33.64
		ATOM	4901		INH V	1	12.194	42.381	65.339	1.00 31.88
	5	ATOM	4902		INH V	1	11.928	41.198	66.028	1.00 31.07
		ATOM	4903		INH V	1	10.630	40.858	66.412	1.00 28.70
10		MOTA	4904		INH V	1	13.587	42.710	64.882	1.00 32.51
		ATOM	4905		INH V	1	14.260	41.560	64.121	1.00 34.69
		ATOM	4906		INH V	1	15.683	41.849	63.754	1.00 28.88
	10	MOTA	4907	S1	INH V	1	16.605	40.755	64.790	1.00 29.16
		ATOM	4908	N1	INH V	1	13.497	40.805	63.099	1.00 30.69
		ATOM	4909	0	HOH W	1	44.463	49.888	77.523	1.00 46.91
		ATOM	4910	0	HOH W	2	13.469	27.803	78.018	1.00 20.07
15	1.5	ATOM	4911	0	HOH W	3	4.225	69.721	58.393	1.00 27.76
	15	MOTA	4912	0	HOH W	4	15.603	28.826	61.823	1.00 22.81
		ATOM	4913	0	HOH W	5	22.862	26.624	42.874	1.00 53.05
		ATOM	4914	0	HOH W	6	8.423	46.452	57.584	1.00 32.22
		ATOM	4915	0	HOH W	7	17.904	46.550	68.524	1.00 31.91
		ATOM	4916	О	HOH W	8	22.979	45.895	83.716	1.00 39.37
	20	ATOM	4917	0	HOH W	9	17.707	39.158	55.643	1.00 25.27
20		ATOM	4918	0	HOH W	10	12.439	36.303	59.209	1.00 31.46
		MOTA	4919	0	HOH W	11	17.367	62.730	50.320	1.00 37.74
		ATOM	4920	0	HOH W	12	42.823	52.642	90.552	1.00 53.80
		ATOM	4921	0	HOH W	13	34.337	45.508	97.419	1.00 57.99
	25	ATOM	4922	ō	HOH W	14	6.726	27.119	48.459	1.00 62.29
		ATOM	4923	ō	HOH W	15	-0.093	30.159	71.746	1.00 29.96
		ATOM	4924	ŏ	HOH W	16	-19.673	44.016	58.682	1.00 58.64
25		ATOM	4925	ō	HOH W	17	16.563	26.790	80.837	1.00 38.62
		ATOM	4926	ō	HOH W	18	10.281	35.677	88.518	1.00 26.01
	30	ATOM	4927	ō	HOH W	19	20.973	35.691	44.774	1.00 49.50
	30	ATOM	4928	ŏ	HOH W	20	0.996	19.571	53.713	1.00 49.30
		ATOM	4929	ŏ	HOH W	21	20.424	37.014	85.845	1.00 37.33
		ATOM	4930	ŏ	HOH W	22	-2.498	35.905	53.781	1.00 51.70
		ATOM	4931	ŏ	HOH W	23	39.807	49.718	92.595	
30	35	ATOM	4932	Ö	HOH W	24	16.431	58.267	93.127	1.00 37.39
	33	ATOM	4933	Ö	HOH W	25		45.104		1.00 47.45
		ATOM	4934	Ö	HOH W	26	6.935 40.479		66.012 100.253	1.00 18.12
		ATOM	4935	ŏ	HOH W	27	22.369			1.00 28.72
			4936	0		28		40.324	67.919	1.00 46.36
	40	MOTA	4937		HOH W		37.289	49.457	68.016	1.00 61.37
	40	MOTA	4937	0	HOH W	29	2.611	35.015	55.709	1.00 24.45
35		ATOM		0	HOH W	30	41.088	62.590	98.644	1.00 65.38
		MOTA	4939	0	HOH W	31	17.369	55.024	87.465	1.00 24.22
		ATOM	4940	0	HOH W	32	25.433	20.198	55.692	1.00 44.61
	45	MOTA	4941	0	HOH W	33	3.890	42.770	66.651	1.00 22.34
	43	ATOM	4942	0	HOH W	34	3.934	63.391	62.592	1.00 60.69
		ATOM	4943	0	HOH W	35	22.280	41.610	86.289	1.00 74.20
		MOTA	4944	0	HOH W	36	22.631	46.401	90.078	1.00 47.44
40		ATOM	4945	0	HOH W	37	33.442	20.227	64.569	1.00 55.41
	50	MOTA	4946	0	HOH W	38	39.834	28.974	75.602	1.00 41.72
	50	MOTA	4947	0	HOH W	39	35.232	47.140	54.186	1.00 37.08
		MOTA	4948	0	HOH W	40	36.003	57.784	57.893	1.00 43.05
		MOTA	4949	0	HOH W	41	37.216	27.438	74.564	1.00 50.79
		MOTA	4950	0	HOH W	42	17.770	67.012	77.183	1.00 45.78
45	E E	ATOM	4951	0	HOH W	43	5.341	31.286	78.127	1.00 25.34
45	55	MOTA	4952	0	HOH W	44	33.535	32.503	52.063	1.00 56.13
		MOTA	4953	0	HOH W	45	25.477	33.146	44.610	1.00 65.43
		MOTA	4954	0	HOH W	46	16.235	37.438	52.628	1.00 32.10
		MOTA	4955	0	HOH W	47	28.791	14.101	63.316	1.00 46.67
		ATOM	4956	0	HOH W	48	10.230	24.992	86.967	1.00 38.63
	60	MOTA	4957	0	HOH W	49	30.821	38.856	79.630	1.00 40.44
50		MOTA	4958	0	HOH W	50	12.621	37.226	62.944	1.00 26.70
50		ATOM	4959	0	HOH W	51	27.987	30.609	66.612	1.00 33.55
		MOTA	4960	0	HOH W	52	34.459	28.696	64.242	1.00 51.01
		ATOM	4961	0	HOH W	53	34.969	62.270	91.179	1.00 68.20

5		ATOM	4962	0	HOH W	54	33.631	30.717	62.396	1.00 41.64
		ATOM	4963	ō	HOH W	55	43.987	48.530	91.269	1.00 50.99
		ATOM	4964	ō	HOH W	56	23.412	28.584	85.186	1.00 69.23
		ATOM	4965	ō	HOH W	57	39.834	28.057	72.257	1.00 81.00
	5	ATOM	4966	ō	HOH W	58	2.892	25.685	69.907	1.00 38.96
	•	ATOM	4967	ō	HOH W	59	10.284	47.120	72.671	1.00 40.28
		ATOM	4968	Ö	HOH W	60	32.645	39.037	76.746	1.00 21.71
10		ATOM	4969	ö	HOH W	61	43.535	48.019	95.228	1.00 37.69
		ATOM	4970	ŏ	HOH W	62	11.991	51.053	43.479	1.00 41.05
	10	MOTA	4971	ŏ	HOH W	63	18.329	56.527	89.388	1.00 28.51
	10	ATOM	4972	ŏ	HOH W	64	16.555	9.309	68.875	1.00 89.05
		MOTA	4973	Ö	HOH W	65	23.741	44.759		1.00 38.43
		ATOM	4974	Ö					73.150 41.239	1.00 55.25
			4975	Ö	HOH M	66 67	19.093	53.805	56.933	
15	15	ATOM	4976	Ö	HOH W	67	31.750	60.369		1.00 92.26
	13	ATOM ATOM	4977		HOH W	68 69	24.836 -21.014	68.428 19.446	80.926	1.00 59.25 1.00 52.24
				0	HOH W		· ·		48.342	
		ATOM	4978	0	HOH W	70	11.318	68.028	86.566	1.00 77.81
		ATOM	4979	0	HOH W	71	5.312	60.076	63.511	1.00 36.83
	20	MOTA	4980	0	HOH W	72	7.689	20.219	84.680	1.00 32.24
	20	ATOM	4981	0	HOH W	73	34.988	44.708	64.746	1.00 40.73
20		ATOM	4982	0	HOH W	74	10.614	49.644	41.337	1.00 38.90
		MOTA	4983	0	HOH W	75	19.349	42.973	64.739	1.00 54.53
		MOTA	4984	0	нон w	76	35.916	30.862	80.753	1.00 55.38
		MOTA	4985	0	HOH W	77	9.666	26.046	46.603	1.00 40.09
	25	MOTA	4986	0	HOH W	78	-10.171	46.751	60.237	1.00 29.78
		MOTA	4987	0	нон м	79	46.751	58.883	86.875	1.00 35.92
		MOTA	4988	0	HOH W	80	19.320	32.528	51.000	1.00 33.36
25		MOTA	4989	0	HOH W	81	28.815	39.568	66.176	1.00 59.19
		MOTA	4990	0	HOH W	82	38.207	35.773	73.585	1.00 17.81
	30	ATOM	4991	0	HOH W	83	23.802	33.925	75.175	1.00 25.19
		MOTA	4992	0	HOH W	84	42.241	51.290	99.896	1.00 15.88
		ATOM	4993	0	HOH W	85	3.751	36.678	58.842	1.00 24.97
		ATOM	4994	0	HOH W	86	-7.009	40.341	62.580	1.00 25.39
		ATOM	4995	0	HOH W	87	11.735	58.910	68.155	1.00 39.70
30	35	ATOM	4996	0	нон w	88	13.986	52.835	42.224	1.00 50.91
		ATOM	4997	0	HOH W	89	1.452	46.541	69.459	1.00 35.03
		ATOM	4998	0	HOH W	90	-1.938	55.310	56.971	1.00 28.10
		MOTA	4999	0	HOH W	91	13.801	66.947	52.600	1.00 38.65
		ATOM	5000	0	HOH W	92	21.594	47.218	79.203	1.00 30.31
	40	ATOM	5001	0	HOH W	93	10.639	58.632	90.827	1.00 43.78
25		ATOM	5002	0	HOH W	94	33.335	53.550	68.086	1.00 37.04
35		ATOM	5003	0	HOH W	95	-1.984	28.738	60.212	1.00 31.56
		ATOM	5004	0	HOH W	96	-4.958	51.055	59.250	1.00 34.00
		ATOM	5005	ō	HOH W	97	17.610	39.701	51.503	1.00 28.27
	45	ATOM	5006	o	HOH W	98	10.686	54.166	67.565	1.00 37.68
	• •	ATOM	5007	ō	HOH W	99	20.567	43.859	78.621	1.00 41.57
		ATOM	5008	ō	HOH W		7.013	22.332	69.109	1.00 28.72
40		ATOM	5009	ŏ	HOH W		10.097	53.225	78.477	1.00 35.68
70		ATOM	5010	ŏ	HOH W		10.849	31.404	53.014	1.00 32.22
	50	ATOM	5011	ŏ	HOH W		42.381	59.035	94.728	1.00 36.00
	50	ATOM	5012	ŏ	HOH W		17.234		54.082	1.00 33.65
		ATOM	5012	ŏ	HOH W		26.902	62.025	81.989	1.00 33.03
		ATOM	5014	ŏ	HOH W		-14.313			
		ATOM	5015	ő	HOH W		41.646	49.559	56.204 101.015	1.00 54.36 1.00 68.12
45	55									
70	رر	MOTA	5016	0	HOH W		26.759	43.000	47.219	1.00 32.69
		ATOM	5017	0	HOH W		16.624	48.119	46.545	1.00 38.64
		MOTA	5018	0	HOH W		26.159	32.793	75.230	1.00 24.77
		ATOM	5019	0	HOH W		2.101	33.468	67.006	1.00 31.50
	(0	ATOM	5020	0	HOH W		38.114	36.374	87.451	1.00 44.06
	60	MOTA	5021	0	HOH W		13.211	29.810	61.356	1.00 33.81
50		MOTA	5022	0	HOH W		-3.064	37.863	40.673	1.00 37.92
50		MOTA	5023	0	HOH W		15.007	47.948	69.488	1.00 28.23
		MOTA	5024	0	HOH W		27.101	66.633	80.518	1.00 41.24
		ATOM	5025	0	HOH W	117	11.870	38.304	43.174	1.00 40.85

5		MOTA	5026	0	нон w 118	-13.844	25.597	58.258	1.00 53.75
		ATOM	5027	ō	HOH W 119	2.929	41.135	59.858	1.00 36.49
		ATOM	5028	ō	HOH W 120	24.890	45.490	82.167	1.00 41.65
		ATOM	5029	ŏ	HOH W 121	36.062	59.335	75.090	1.00 38.82
	5	ATOM	5030	ō	HOH W 122	-10.715	32.037	61.699	1.00 78.82
	-	MOTA	5031	ō	HOH W 123	-2.646	25.492	60.812	1.00 48.40
40		ATOM	5032	Ō	HOH W 124	-8.948	46.831	63.556	1.00 48.06
10		ATOM	5033	0	HOH W 125	-17.843	39.367	36.020	1.00 35.80
		ATOM	5034	0	HOH W 126	2.218	57.766	62.253	1.00 44.61
	10	ATOM	5035	0	HOH W 127	10.736	62.766	64.366	1.00 55.84
		ATOM	5036	0	HOH W 128	0.884	35.562	63.963	1.00 44.14
		MOTA	5037	0	HOH W 129	19.165	59.557	60.644	1.00 47.82
		ATOM	5038	0	HOH W 130	1.546	27.875	68.443	1.00 39.69
15		MOTA	5039	0	HOH W 131	5.497	26.285	76.668	1.00 44.47
	15	MOTA	5040	0	HOH W 132	14.505	36.538	88.996	1.00 40.00
		ATOM	5041	0	HOH W 133	.8.534	28.713	88.519	1.00 46.55
		ATOM	5042	0	HOH W 134	6.125	45.267	77.959	1.00 45.57
		ATOM	5043	0	HOH W 135	26.016	18.543	78.878	1.00 51.65
		ATOM	5044	0	HOH W 136	33.880	23.025	70.739	1.00 46.95
	20	ATOM	5045	0	HOH W 137	19.230	26.073	49.998	1.00 51.97
20		ATOM	5046	0	HOH W 138	41.563	41.085	77.326	1.00 43.14
		ATOM	5047	0	HOH W 139	39.187	63.067	75.380	1.00 56.52
		ATOM	5048	0	HOH W 140	26.878	54.491	67.203	1.00 42.14
	25	ATOM	5049	0	HOH W 141	22.988	62.189	74.174	1.00 48.31
	25	ATOM	5050	0	HOH W 142	25.190	62.803	71.067	1.00 67.16
		ATOM	5051	0	HOH W 143	18.598	45.126	81.949	1.00 53.80
25		ATOM	5052	0	HOH W 144	19.782 21.735	53.129	90.556	1.00 48.73
20		MOTA MOTA	5053 5054	0	HOH W 145 HOH W 146	25.707	48.367 57.012	86.454 93.476	1.00 40.39
	30		5055	0	HOH W 147	22.832	62.085		1.00 53.61
	30	ATOM ATOM	5056	Ö	HOH W 147	25.725	67.203	93.149 89.990	1.00 46.02 1.00 75.23
		MOTA	5050	ŏ	HOH W 149	10.773	53.653	85.697	1.00 50.65
		ATOM	5058	Ö	HOH W 150	4.221	58.449	86.608	1.00 30.63
		ATOM	5059	o	HOH W 151	7.790	72.096	84.410	1.00 49.23
30	35	ATOM	5060	ő	HOH W 152	2.387	58.282	67.835	1.00 33.29
	23	ATOM	5061	Ö	HOH W 153	0.921	49.551	69.095	1.00 59.60
		ATOM	5062	ŏ	HOH W 154	8.722	45.171	71.561	1.00 46.56
		ATOM	5063	ō	HOH W 155	6.422	47.947	81.081	1.00 57.56
		ATOM	5064	0	HOH W 156	15.936	56.908	55.129	1.00 43.33
	40	ATOM	5065	0	HOH W 157	3.032	19.635	62.453	1.00 80.38
35		ATOM	5066	0	HOH W 158	-4.228	58.058	47.057	1.00 39.66
33		MOTA	5067	0	HOH W 159	1.197	41.002	78.942	1.00 57.22
		MOTA	5068	0	HOH W 160	1.259	43.651	68.100	1.00 37.94
		MOTA	5069	0	HOH W 161	25.799	64.833	56.690	1.00 38.96
	45	MOTA	5070	0	HOH W 162	-11.853	45.054	45.070	1.00 38.38
		ATOM	5071	0	HOH W 163	40.159	31.033	78.548	1.00 75.36
		ATOM	5072	0	HOH W 164	21.477	20.377	79.349	1.00 35.96
40		MOTA	5073	0	HOH W 165	26.347	44.558	72.803	1.00 42.21
	50	MOTA	5074	0	HOH W 166	16.446	61.207	59.687	1.00 39.70
	50	MOTA	5075	0	HOH W 167	27.695	64.216	82.410	1.00 44.71
		ATOM	5076		HOH W 168	-2.998	57.511	34.738	1.00 45.35
		ATOM	5077	0	HOH W 169	6.608	51.527	60.826	1.00 39.48
		MOTA	5078	0	HOH W 170	31.104	28.934	81.337	1.00 43.19
45		ATOM	5079	0	HOH W 171	10.135	28.233	45.533	1.00 41.24
45	55	ATOM	5080	0	HOH W 172	8.201	43.960	75.322	1.00 37.71
		ATOM	5081	0	HOH W 173	13.799	66.601	85.597	1.00 34.74
		ATOM	5082	0	HOH W 174	16.664	53.670	65.006	1.00 43.69
		ATOM	5083	0	HOH W 175	18.301	47.296	43.793	1.00 45.84
	60	ATOM	5084	0	HOH W 176	11.717	61.868	52.648	1.00 34.93
	60	ATOM	5085	0	HOH W 177	29.516	23.822	76.838	1.00 51.50
50		ATOM	5086	0	HOH W 178	39.940	60.509	78.535	1.00 46.33
		ATOM	5087	0	HOH W 179	-1.803 7.343	44.974	37.278	1.00 52.56
		ATOM	5088	0	HOH W 180	7.343	47.305	65.468	1.00 47.27
		ATOM	5089	0	HOH W 181	17.912	15.338	81.793	1.00 50.08

Control of the Contro

5		ATOM	5090	0	HOH W 182	-4.631	55.917	82,183	1.00 65.36
		MOTA	5091	0	HOH W 183	32.973	42.656	86.667	1.00 43.97
		MOTA	5092	0	HOH W 184	-1.834	36.784	71.040	1.00 45.10
	_	MOTA	5093	0	HOH W 185	-4.519	34.633	71.838	1.00 43.99
	5	MOTA	5094	0	HOH W 186	4.518	68.554	71.661	1.00 46.99
		MOTA	5095	0	HOH W 187	2.774	37.503	61.490	1.00 45.81
40		ATOM	5096	0	HOH W 188	31.770	43.526	51.410	1.00 58.02
10		MOTA	5097	0	HOH W 189	5.471	43.861	38.891	1.00 49.43
	10	ATOM	5098	0	HOH W 190	11.934	58.219	70.811	1.00 49.96
	10	ATOM	5099	0	HOH W 191	33.112	26.203	70.484	1.00 60.03
		MOTA MOTA	5100 5101	0	HOH W 192 HOH W 193	30.914 0.400	43.017	70.613	1.00 73.23
		ATOM	5102	Ö	HOH W 194	48.247	39.300 56.159	39.714 86.370	1.00 65.37 1.00 60.09
		ATOM	5103	ŏ	HOH W 195	12.359	59.992	62.698	1.00 53.57
15	15	ATOM	5104	ŏ	HOH W 196	11.149	17.504	78.264	1.00 54.43
		ATOM	5105	ō	HOH W 197	-4.284	31.953	60.991	1.00 34.43
		MOTA	5106	0	HOH W 198	29.888	35.624	82.772	1.00 52.16
		ATOM	5107	0	HOH W 199	14.388	39.115	89.656	1.00 47.93
		ATOM	5108	0	HOH W 200	-8.529	51.475	47.745	1.00 61.00
	20	ATOM	5109	0	HOH W 201	-15.572	53.338	52.008	1.00 72.42
20		ATOM	5110	0	HOH W 202	24.319	38.590	87.128	1.00 50.03
20		MOTA	5111	0	HOH W 203	25.366	70.670	82.839	1.00 49.01
		ATOM	5112	0	HOH W 204	18.531	27.749	86.236	1.00 48.64
	25	ATOM	5113	0	HOH W 205	21.694	20.030	81.796	1.00 49.04
	25	ATOM	5114	0	HOH W 206	23.953	47.993	67.580	1.00 40.39
		ATOM	5115	0	HOH W 207	22.012	40.217	90.228	1.00 42.29
		ATOM	5116	0	HOH W 208	16.197	45.094	43.427	1.00 48.00
25		ATOM ATOM	5117 5118	0	HOH W 209 HOH W 210	21.019	68.985	84.382	1.00 56.50
	30	ATOM	5119	ŏ	HOH W 211	-7.134 40.843	33.015 44.050	71.591	1.00 56.31
	50	ATOM	5120	ŏ	HOH W 211	20.374	14.856	89.284 56.642	1.00 43.07
		ATOM	5121	ŏ	HOH W 213	12.723	46.277	73.748	1.00 50.07 1.00 59.15
		ATOM	5122	ō	HOH W 214	8,956	43.704	58.706	1.00 45.56
		ATOM	5123	Ō	HOH W 215	-2.433	36.012	80.232	1.00 54.12
30	35	ATOM	5124	0	HOH W 216	5.257	25.271	55.914	1.00 53.23
		ATOM	5125	0	HOH W 217	13.354	64.403	53.862	1.00 47.27
		ATOM	5126	0	HOH W 218	30.477	42.517	67.472	1.00 48.17
		ATOM	5127	0	HOH W 219	14.139	47.479	76.123	1.00 79.04
	40	ATOM	5128	0	HOH W 220	0.829	29.563	50.769	1.00 48.10
	40	ATOM	5129	0	HOH W 221	32.979	51.667	96.624	1.00 51.30
35		ATOM	5130	0	HOH W 222	14.677	45.948	71.756	1.00 52.31
33		ATOM	5131	0	HOH W 223	33.890	24.505	58.094	1.00 43.65
		ATOM ATOM	5132 5133	0	HOH W 224	17.853	9.519	65.560	1.00 55.94
	45	ATOM	5134	Ö	HOH W 225 HOH W 226	37.794 29.206	31.473 50.335	62.305	1.00 50.38
		ATOM	5135	ŏ	HOH W 227	4.932	48.808	62.673 63.354	1.00 45.43 1.00 42.45
		ATOM	5136	ŏ	HOH ₩ 228	18.933	59.070	55.899	1.00 42.43
		ATOM	5137	Ō	HOH ₩ 229	13.849	18.833	83.641	1.00 55.89
40		MOTA	5138	0	HOH W 230	25.919	46.022	68.076	1.00 35.63
	50	ATOM	5139	0	HOH W 231	27.565	65.098	75.153	1.00 73.11
		ATOM	5140	0	HOH W 232	27.128	39.012	68.497	1.00 40.77
		ATOM	5141	0	HOH W 233	40.706	52.468	74.641	1.00 51.60
		MOTA	5142	0	HOH W 234	21.689	65.312	58.080	1.00 66.72
	EE	ATOM	5143	0	HOH W 235	9.121	17.615	59.271	1.00 51.98
45	55	ATOM	5144	0	HOH W 236	17.931	36.565	88.091	1.00 54.77
		ATOM	5145	0	HOH W 237	33.843	36.707	52.576	1.00 61.60
		ATOM	5146	0	HOH W 238	-3.693	50.074	63.986	1.00 43.64
		MOTA	5147	0	HOH W 239	44.272	44.279	81.461	1.00 69.21
	60	MOTA MOTA	5148 5149	0	HOH W 240	2.092	28.868	52.894	1.00 54.01
	00	MOTA	5150	0	HOH W 241 HOH W 242	8.309	33.518	71.442	1.00 68.05
50		ATOM	5150	Ö	HOH W 243	1.051 44.255	31.947 51.162	69.204 96.650	1.00 52.88
55		ATOM	5152	Ö	HOH W 244	16.173	45.408	46.636	1.00 20.00 1.00 20.00
		ATOM	5153	ŏ	HOH W 245	41.130	50.734		1.00 20.00
				-		-1.100	50.754	211331	1.00 20.00

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5		MOTA	5154	0	HOH W 246	36.912	36.263	75.911	1.00 20.00
		MOTA	5155	0	HOH W 247	-17.107	27.146	54.728	1.00 20.00
		MOTA	5156	0	HOH W 248	24.078	46.307	79.123	1,00 20,00
		ATOM	5157	0	HOH W 249	-12.250	47.964	61.593	1.00 20.00
	5	ATOM	5158	0	HOH W 250	35.804	51.343	51.682	1.00 20.00
		MOTA	5159	0	HOH W 251	25.537			1.00 20.00
		ATOM	5160	0	HOH W 252	0.539	55.427	62.088	1.00 20.00
10		END							

Claims

CLAIMS

An isolated protein comprising at least a subsequence of the amino acid sequence of LTA₄ hydrolase, which exhibits a three-dimensional form essentially as disclosed in Table 9 by the parameters defining atom 1 to atom 4876, said subsequence being capable of participating in the control of the an enzymatic pathway, such as the leukotriene cascade, or a functionally equivalent part, derivative or conformational analogue thereof.

2. A protein according to claim 1, which comprises an enzymatically active site defined in the following table:

	Left wall	Right wall
1		Lys608, Asp606, Lys605,
<u></u>		Lys354, Thr355
2	Phe356, Phe362	Gln544, Asp573, Lys572, Arg568
3	Val376	Lys565, Arg540, Leu507
4	Ser380, Ser352, Glu348	Pro569
5	Tyr378, Glu348	Arg563, Glu533, Phe536, Arg537, Tyr267
6	Tyr383, Phe314, Glu318, Glu384, Arg326	
7	Gly268, Gly269, Met270	His295, Asn341, Phe340
8	Ser288, His497	Glu325, Asn291

- 3. A protein according to claim 2, which is an enzyme having a metallohydrolase activity capable of participating in the regulation of enzyme activities in biochemical pathways, wherein said enzymes have structures similar to the ones defined in claim 2.
- 4. A protein according to claim 1, which comprises an enzymatically active site defined by the following amino acids: Gln136; Ala137; Tyr267; Gly268; Gly269; Met270; Glu271; Val292; His295; Glu296; His299; Glu318; Tyr378; Tyr383; Arg563; Lys565.
- A protein according to claim 1, which comprises an enzymatically active site defined by the following amino acids: Gln136; Ala137; Tyr267; Gly268; Gly269; Met270; Glu271; Val292; His295; Glu296; His299; Trp315; Glu318; Val322;

5 Phe362; Val367; Leu369; Pro374; Asp375; Ile372; Ala377; Pro382; Tyr378; Tyr383; Arg563; Lys565. 6. A compound which is substantially complementary to a protein according to any one of claims 1-5. 10 5 7. A compound according to claim 6, which is substantially complementary to an enzymatically active site of said protein and which is capable of specifically inhibiting said enzymatic activity. 15 8. A compound according to claim 7, which is an inhibitor of a metallohydrolase enzyme. 9. An isolated complex, which is comprised of a protein according to claim 1-5 and 10 20 a complementary compound according to any one of claims 6-8, wherein the three-dimensional structure of LTA4 hydrolase is essentially as disclosed in Table 9 by the parameters defining atom 1- atom 4876, or a functionally equivalent 25 part, derivative or conformational analogue of such a complex. 15 10. A complex according to claim 9, wherein the protein complexed with LTA₄ hydrolase is selected from the group which consists of bestatin, thiolamine or hydroxamic acid, or a functionally equivalent part, derivative or conformational 30 analogue of such a complex. 11. Use of the parameters of a protein according to any one of claims 1-5, a com-20 pound according to any one of claims 6-8 or a complex according to claim 9 or 35 10 in drug design, such as in molecular modeling, direct structure-based design and/or combinatorial chemistry. 12. Use according to claim 11, wherein said parameters are selected from the pa-40 rameters disclosed in Table 9 defining atom 1- atom 4876. 25 13. Use according to claim 11 or 12, wherein said drug is for the treatment and/or prevention of disorders involving acute and chronic inflammatory and/or allergic 45 symtoms, said disorder being selected from the group consisting of arthritis, inflammatory bowel disease (IBD), psoriasis, chronic obstructive pulmonary disease (COPD), and acquired immune deficiency syndrome (AIDS). 50 14. Use according to claim 11 or 12, wherein said drug is for the treatment and/or 30 prevention of proliferative disorders, such as neoplasias and/or cancer.

5		15. Use according to claim 11 or 12, wherein said drug is for the treatment and/or
		prevention of disorders caused by the lethal factor of <i>Bacillus anthracis</i> , e.g. anthrax.
10		16. A method for screening LTA ₄ hydrolase analogues that mimic at least a part of
10	5	-
	J	the three dimensional structure of the LTA ₄ hydrolase molecule as defined by the
		parameters shown in Table 9 for atom 1 to atom 4876, which comprises the steps
15		of
		(a) producing a multiplicity of analogue structures of LTA ₄ hydrolase and
		(b) selecting an analogue structure, wherein the three-dimensional configuration and
20	10	spatial arrangement of one or more enzymatically active sites and/or binding sites
		of said LTA ₄ hydrolase remain substantially preserved.
		17. A method according to claim 16, wherein an analogue exhibiting an enzymatic
		activity, such as an epoxide hydrolase and/or aminopeptidase activity, is selected.
25		18. A method according to claim 16 or 17, wherein an enzymatic inhibitor comple-
	15	mentary to the amino acids defined in any one of claims 3, 4 or 5 is screened for.
		19. An analogue obtainable by the method according to any one of claims 16-18.
30		20. An analogue according to claim 19, which exhibits an increased catalytic activ-
		ity when compared to the naturally occurring form of LTA4 hydrolase, such as
		defined in Table 9 by parameters of atom 1 to atom 4876.
35	20	21. A method for screening LTA ₄ hydrolase binding compounds complementary to
		a region of LTA ₄ hydrolase, preferably an enzymatically active site thereof,
		which comprises the steps of
		(a) producing a multiplicity of possible complementary structures and
40		(b) selecting a structure, wherein the three-dimensional configuration and spatial ar-
	25	rangement of regions involved in binding to LTA ₄ hydrolase remain substantially
45		preserved, which selection is based on the three-dimensional structure of LTA ₄
		hydrolase, and/or LTA ₄ hydrolase complexed to an inhibitor thereof, in a form
		adopted thereof in nature, such as defined in Table 9.
50	20	22. A method according to claim 21, wherein a general metallohydrolase inhibitor is
	30	selected, which is capable of inhibiting an enzyme belonging to the M1 family.

5		23. A method according to claim 21, wherein an inhibitor of the epoxide hydrolase
		activity and/or aminopeptidase activity of LTA ₄ hydrolase or of LTC ₄ synthases is selected.
10	5	24. A method according to claim 21, wherein a compound capable of antagonizing LTB ₄ receptor binding of a cell is selected.
	-	25. A compound obtainable by the method according to any one of claims 21-24.
15		26. A method of engineering a protein, which method comprises the steps of
		-identification of a suitable set of mutations based on the structure of LTA ₄ hydrolase;
20	10	-generation of a library of genes which contains the suitable sequence variations;
		-selection of clones encoding the LTA ₄ hydrolase analogues with a desired activity function;
25		wherein said desired activity is the capability of efficiently producing an organic compound of interest.
	15	27. A method according to claim 26, wherein the specified property is the suicidal
		mode of action of LTA ₄ hydrolase.
30		28. A process for the purification of a protein according to any one of claims 1-3 or
		obtained according to claim 26 or 27, which purification includes hydroxyapatite-
		based chromatography and a subsequent anion exchange chromatography.
35	20	29. A process for the crystallisation of an LTA4 hydrolase, an analogue or a deriva-
		tive thereof, wherein said crystallisation is performed with the addition of a yt-
		terbium salt as an additive, such as an ytterbium chloride.
40		30. A protein obtained by the method according to any one of claims 27-29.
		31. A protein according to claim 30, which is present in an essentially pure form.
	25	32. An isolated nucleic acid encoding a protein according to claim 30 or 31.
45		33. A nucleic acid capable of specifically hybridising to a the nucleic acid according
,,,		to claim 32.
		34. Use of a protein, which is a genetically modified LTA4 hydrolase, according to
		claim 30 or 31 in the preparation of LTB ₄ or other metabolites in the leukotriene
50	30	cascade,

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5 35. A protein according to any one of claims 6-8, 25, 30 or 31 for use as a medicament. 36. Use of a protein according to any one of claims 6-8, 25, 30 or 31 in the manufacture of a medicament for the treatment and/or prevention of acute and chronic 10 5 inflammatory and/or allergic disorders, said disorder being selected from the group consisting of arthritis, inflammatory bowel disease (IBD), psoriasis and chronic obstructive pulmonary disease (COPD); neoplasias and/or cancer; or 15 disorders caused by the lethal factor of Bacillus anthracis, e.g. anthrax. 37. Use of a protein according to any one of claims 6-8, 25, 30 or 31, in the manu-10 facture of a medicament for the treatment and/or prevention of an anti-20 inflammatory and/or anti-allergenic disorder, such as bronchial asthma, allergic rhinitis, conjunctivitis etc. 38. Use of a protein according to any one of claims 6-8, 25, 30 or 31 in the manu-25 facture of a medicament for the treatment and/or prevention of infection caused 15 be human immunodeficiency virus (HIV). 30 35 40

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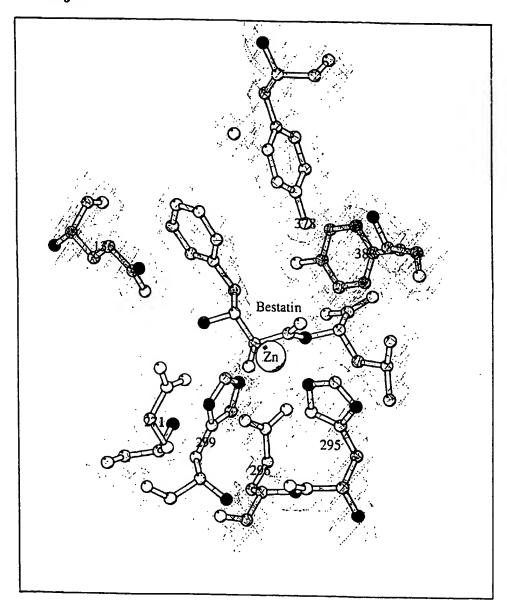
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Figure 1

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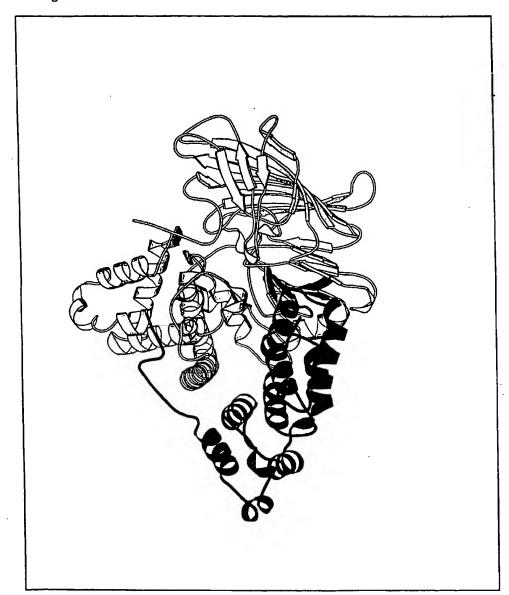
Figure 2



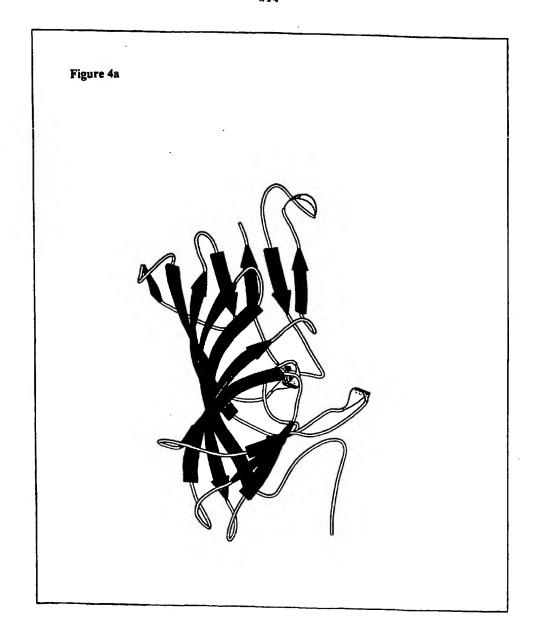
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Figure 3



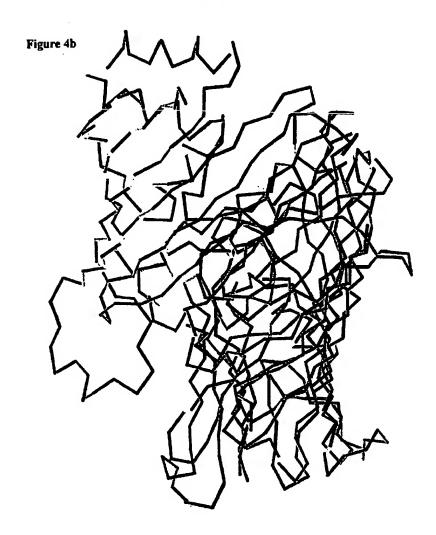
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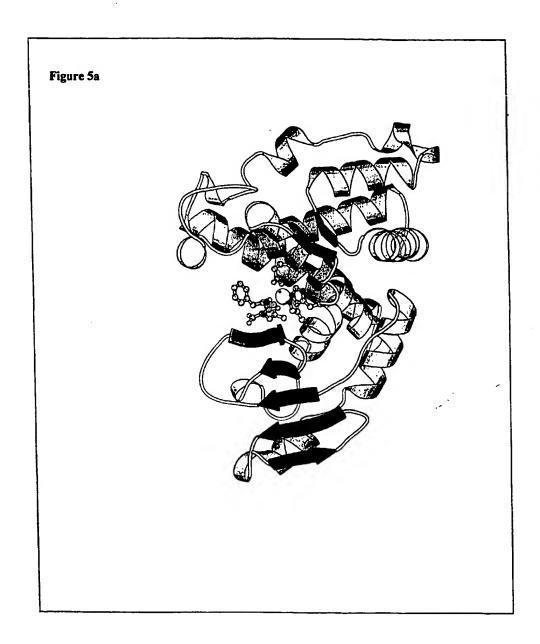
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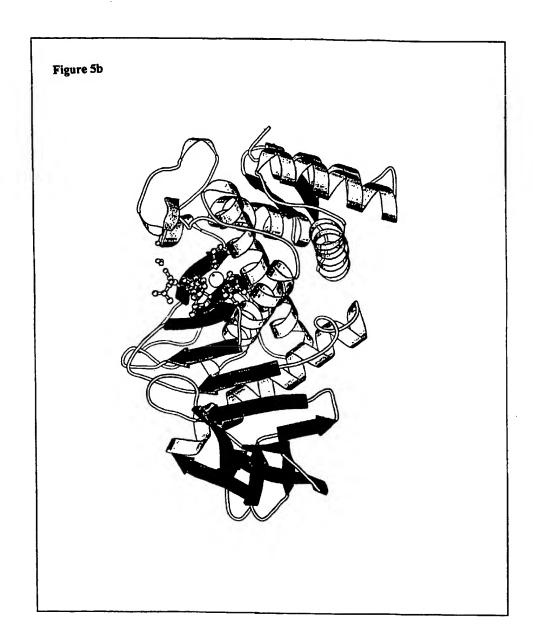


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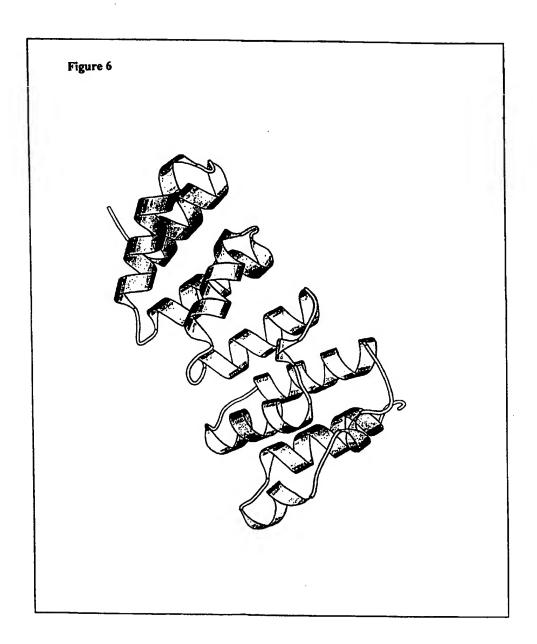


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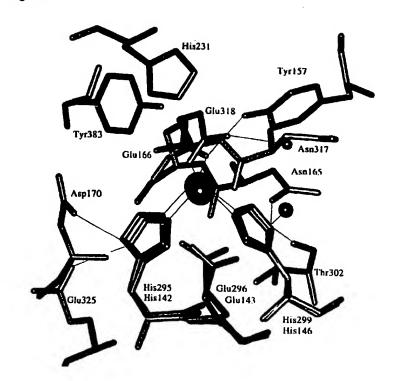
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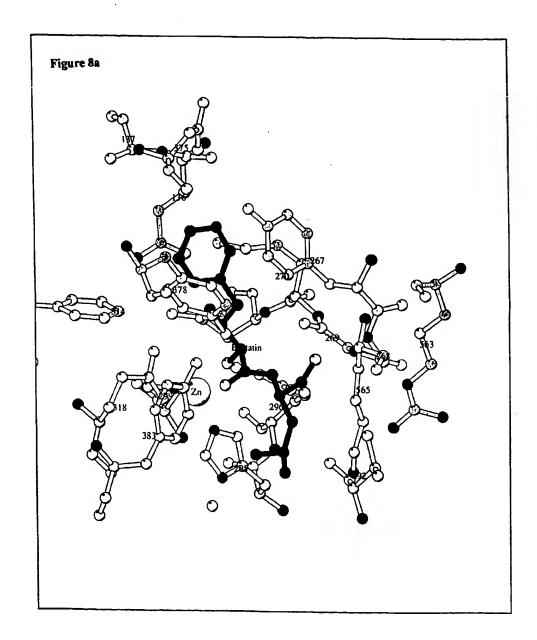
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Figure 7



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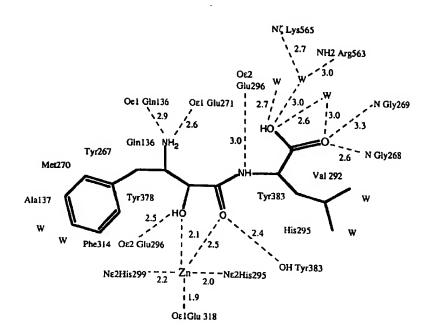
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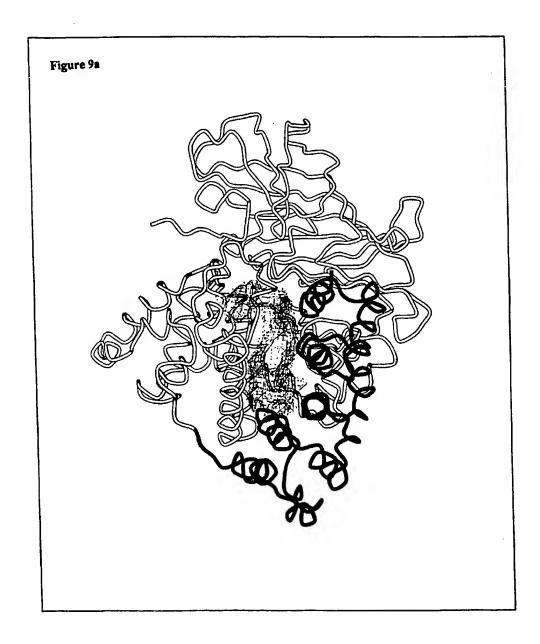
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Figure 8b



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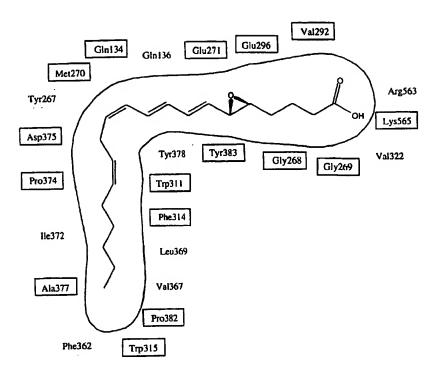
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Figure 9b



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SEQUENCE LISTING

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<110> Haeggström et al., Jesper

<120> DRUG DESIGN BASED ON THE STRUCTURE OF LTA, HYDROLASE

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<170> PatentIn Ver. 2.1

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<213> HUMAN

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<223> AMINO ACID SEQUENCE OF HUMAN LEUKOTRIENE A4
HYDROLASE

<400>

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Cys Arg Thr Lys His Leu His Leu Arg Cys Ser Val Asp Phe Thr Arg 20 25 30

Arg Thr Leu Thr Gly Thr Ala Ala Leu Thr Val Gln Ser Gln Glu Asp 35 40 45

Asn Leu Arg Ser Leu Val Leu Asp Thr Lys Asp Leu Thr Ile Glu Lys
50 55 60

Val Val Ile Asn Gly Gln Glu Val Lys Tyr Ala Leu Gly Glu Arg Gln 65 70 75 80

Ser Tyr Lys Gly Ser Pro Met Glu Ile Ser Leu Pro Ile Ala Leu Ser 85 90 95

Lys Asn Glu Glu Ile Val Ile Glu Ile Ser Phe Glu Thr Ser Pro Lys 100 105 110

Ser Ser Ala Leu Gln Trp Leu Thr Pro Glu Gln Thr Ser Gly Lys Glu 115 120 125

His Pro Tyr Leu Phe Ser Gln Cys Gln Ala Ile His Cys Arg Ala Ile 130 135 140

Leu Pro Cys Gin Asp Thr Pro Ser Val Lys Leu Thr Tyr Thr Ala Glu 145 150 155 160

Val Ser Val Pro Lys Glu Leu Val Ala Leu Met Ser Ala Ile Arg Asp 165 170 175

- Gly Glu Thr Pro Asp Pro Glu Asp Pro Ser Arg Lys Ile Tyr Lys Phe 180 185 190
- Ile Gin Lys Vai Pro Ile Pro Cys Tyr Leu Ile Ala Leu Vai Vai Gly 195 200 205
- Ala Leu Giu Ser Arg Gin Ile Giy Pro Arg Thr Leu Val Trp Ser Glu 210 215 220
- Lys Glu Gln Val Glu Lys Ser Ala Tyr Glu Phe Ser Glu Thr Glu Ser 225 230 235 240
- Met Leu Lys Ile Ala Glu Asp Leu Giy Giy Pro Tyr Val Trp Gly Gln 245 250 255
- Tyr Asp Leu Val Leu Pro Pro Ser Phe Pro Tyr Gly Gly Met Glu 260 265 270
- Asn Pro Cys Leu Thr Phe Val Thr Pro Thr Leu Leu Ala Gly Asp Lys 275 280 285
- Ser Leu Ser Asn Val Ile Ala His Glu Ile Ser His Ser Trp Thr Gly 290 295 300
- Asn Leu Val Thr Asn Lys Thr Trp Asp His Phe Trp Leu Asn Glu Gly 305 310 315 320
- His Thr Val Tyr Leu Glu Arg His Ile Cys Gly Arg Leu Phe Gly Glu 325 330 335
- Lys Phe Arg His Phe Asn Ala Leu Gly Gly Trp Gly Glu Leu Gln Asn 340 345 350
- Ser Val Lys Thr Phe Gly Glu Thr His Pro Phe Thr Lys Leu Val Val 355 360 365
- Asp Leu Thr Asp Ile Asp Pro Asp Val Ala Tyr Ser Ser Val Pro Tyr 370 375 380
- Glu Lys Gly Phe Ala Leu Leu Phe Tyr Leu Glu Gln Leu Leu Gly Gly 385 390 395 400
- Pro Glu Ile Phe Leu Gly Phe Leu Lys Ala Tyr Val Glu Lys Phe Ser 405 410 415
- Tyr Lys Ser Ile Thr Thr Asp Asp Trp Lys Asp Phe Leu Tyr Ser Tyr 420 425 430
- Phc Lys Asp Lys Val Asp Val Leu Asn Gln Val Asp Trp Asn Ala Trp 435 440 445
- Leu Tyr Ser Pro Gly Leu Pro Pro Ile Lys Pro Asn Tyr Asp Met Thr 450 455 460
- Leu Thr Asn Ala Cys lle Ala Leu Ser Gln Arg Trp Ile Thr Ala Lys 465 470 475 480
- Glu Asp Asp Leu Asn Ser Phe Asn Ala Thr Asp Leu Lys Asp Leu Ser

Add to the same of

3

Ser His Gln Leu Asn Glu Phe Leu Ala Gln Thr Leu Gln Arg Ala Pro 500 505 510

Leu Pro Leu Gly His Ile Lys Arg Met Gln Glu Val Tyr Asn Phe Asn 515 520 525

Ala Ile Asn Asn Ser Glu Ile Arg Phe Arg Trp Leu Arg Leu Cys Ile 530 535 540

Gin Ser Lys Trp Glu Asp Ala Ile Pro Leu Ala Leu Lys Met Ala Thr 545 550 555 560

Glu Gln Gly Arg Mct Lys Phe Thr Arg Pro Leu Phe Lys Asp Leu Ala 565 570 575

Ala Phe Asp Lys Ser His Asp Gln Ala Val Arg Thr Tyr Gln Glu His 580 585 590

Lys Ala Ser Met His Pro Val Thr Ala Met Leu Val Gly Lys Asp Leu 595 600 605

Lys Val Asp 610

أجهر أياط والأحوا أحاك الماك الراب والراجون فياي

INTERNATIONAL SEARCH REPORT

International application No.
PCT/SE 00/00384

A. CLASSIFICATION OF SUBJECT MATTER					
IPC7: C12N 9/14, A61K 38/46 // A61P 29/00, A61P 037/08 According to International Patent Classification (IPC) or to both national classification and IPC					
B. FIELDS SEARCHED					
Minimum documentation searched (classification system followed by classification symbols)					
IPC7: C12N, A61K					
Documentat	tion searched other than minimum documentation to the	extent that such documents are included i	n the fields searched		
SE,DK,FI,NO classes as above					
Electronic data base consulted during the international search (name of data base and, where practicable, search terms used)					
C. DOCUMENTS CONSIDERED TO BE RELEVANT					
Category*	Citation of document, with indication, where app	propriate, of the relevant passages	Relevant to claim No.		
X	Pir database, accession no. S659	047,	1-38		
	1996-10-28, Mancini J. A et and characterization of the	human leukotriene			
	A(4) hydrolase gene"; Eur. J 1995	D. Biochem. 231, 65-71,			
x	J. Mol. Biol., Volume 238, 1994,	Uidaaki Tawaa at	120		
^	al, "Crystallization and Pre	liminary X-ray	1-38		
	Crystallographic Studies of Leukotriene A4 Hydrolase Com	Recombinant Human plexed with Bestatin"			
	page 854 - page 856				
			1		
X Furth	er documents are listed in the continuation of Box	C See natent family annu			
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special reason (as specified) "Y" document of particular relevance: the claimed invention cannot be			claimed invention cannot be		
means	ent referring to an oral disclosure, use, exhibition or other	considered to involve an inventive ste combined with one or more other such being obvious to a person skilled in th	a documents, such combination		
"P" document published prior to the international filing date but later than the priority date claimed "&" document member of the same patent family					
Date of the actual completion of the international search		Date of mailing of the international search report			
6 June 2000		2 6 - 06- :	2000		
Name and	mailing address of the ISA/	Authorized officer			
Swedish Patent Office Box 5055, S-102 42 STOCKHOLM Yvonne Stösteen/gh					
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INTERNATIONAL SEARCH REPORT

International application No.
PCT/SE 00/00384

	FCI/3E	JU/UU384
C (Continu	ation). DOCUMENTS CONSIDERED TO BE RELEVANT	
Category*	Citation of document, with indication, where appropriate, of the relevant passage	s Relevant to claim No
x	Proc.Natl.Acad.Sci., Volume 88, 1991, Medina J. F. et al, "Leukotriene A4 hydrolase: Determination of the three zinc-binding ligands by site-directed mutagenesis and zinc analysis" page 7620 - page 7624	4,5
A		1-3,6-38
x	Eur. J. Biochem, Volume 231, 1995, Blomster, Martina et al, "Evidence for a catalytic role of tyrosine 383 in the peptidase reaction of leukotriene A4 hydrolase" page 528 - page 534	4,5
A		1-3,6-38
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